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THE HANDBOOK OF GROUNDWATER ENGINEERING

Editor-in-Chief
Jacques W. Delleur

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Editor

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Dr. Delleur's research has been supported by the U.S. Department of the Interior, the National Science Foundation, the U.S. Department of Transportation and the U.S. Department of Agriculture. He has served as an advisor to the U.S. Geological Survey, is a member of the international board of advisors of the American Society of Civil Engineers (ASCE) *Journal of Hydrologic Engineering* and is a member of the scientific council of the *Revue des Sciences de l'Eau / Journal of Water Science.* He served as a reviewer for the National Science Foundation, and for the scientific journals *Water Resources Research, Journal of Hydrology, Journal of the American Water Resources Association,* and the *Journal of Hydraulics.* He is a fellow of the Indiana Academy of Sciences, received the 1961 Freeman Fellow Award of the ASCE, in 1983 received an NSF/CNRS US-France Senior Scientist Exchange Award, and in 1992 received the Charles Harold Bechert Award of the Indiana Water Resources Association for significant contribution to the water resources profession in Indiana. While on sabbatical leave, Dr. Delleur did research in hydrology at the French National Hydraulics Laboratory (1968-69 and 1976-77), at the University of Grenoble, France (1961-62 and 1983-84) and at the Vrije Universiteit Brussel (Free University of Brussels), Belgium (1991). He has been a guest lecturer at the Ecole Polytechnique Fédérale de Lausanne (Federal Polytechnic School of Lausanne), Switzerland, at the Free University of Brussels, Belgium, at Imperial College in London, at the University of Tokushima, Japan, at the Indian Institute of Technology in Kanpur, India, at the Mahommadia School of Engineering in Rabat, Morocco, at the Taiwan National University in Taipei, Taiwan, and at the Universidad de los Andes (University of the Andes) in Bogota, Colombia.

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marching algorithms. A correction can then be implemented in the next step depending on the deviation of the interacting variables. Furthermore, this simulation-based approach offers the only way to address the promising avenues of merging different treatment technologies into integrated treatment systems that achieve enhanced productivity and efficiency (treatment time, cost, and clean up level).

Specific steps for an efficient implementation of the macroengineering approach are:

- Better coordinate soil data collection with simulation of interaction processes for prediction needs.
- Hierarchically organize space and time scales of field measurements of interaction phenomena and corresponding media properties and attendant models
- Place more emphasis on the scientific understanding (prediction) of physicochemical processes rather than relying solely on data collection
- Use integrated simulation tools to better identify combinations of treatment processes as they interact with the soil media

References

ZEi, 1994-1997, Environmental Information System (EIS) Graphical Platform, Documentation:
EIS Installation Guide, Mi-96-G001.
EIS User's Guide, Mi-96-G002.
EIS Theoretical Manual, Mi-96-M010.
EIS Automated Generalized Kriging Procedures, Mi-96-M011.
EIS-Biorem3D - Modeling Intrinsic Remediation, Mi-96-M012.
EIS-BioQuick- Quick Model for IR, Mi-96-M013.
EIS-Raw Data Base, Mi-96-M014.

Goodchild, M. F. 1991. Spatial analysis with GIS: Problems and Prospects. Proceedings, GIS/LIS '91, vol. 1, 40-48. Bethesda: American Congress on Surveying and Mapping, Bethesda, MD.

Egenhofer, M. J. and Frank, A. U. 1992. Object-oriented modeling for GIS. *URISA Journal* 4(2):3-19, London.

Konikow, L. F. and Bredehoeft, J. D. 1978. Computer model of two-dimensional solute transport and dispersion in groundwater, *Techniques of Water Resources Investigations*, Book 7, Chap. C2, U.S. Geological Survey, Reston, Virginia.

Properties of Soil-water, Soil-Gas, Soil-Contaminant under EIS, Mi-96-D001.

20

Groundwater Modeling

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20.1 Introduction

Effective management of groundwater requires the ability to predict subsurface flow and transport of solutes, and the response of fluid and solute flux to changes in natural or human-induced stresses. One popular type of tool that has been evolving since the mid-1960s is the deterministic, distributed-parameter, computer simulation model for analyzing flow and solute-transport in groundwater systems. The development of the computer simulation model has somewhat paralleled the development and increasing availability of faster, larger memory, more capable, yet less expensive computer systems.

The purpose of this chapter is to review the state of the art in deterministic modeling of groundwater flow and transport processes. This chapter, based largely on Konikow (1996), is aimed at practitioners and is intended to describe the types of models that are available and how they may be applied to complex field problems. It will discuss the philosophy and theoretical basis of deterministic modeling, the advantages and limitations of models, the use and misuse of models, how to select a model, and how to calibrate and evaluate a model. However, as this chapter is only a review, it cannot offer comprehensive and in-depth coverage of this complex topic; instead, it guides the reader to references that provide more details.

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20.2 Models

The word *model* has so many definitions and is so overused that it is sometimes difficult to discern its meaning (Konikow and Bredehoeft, 1992). A model is perhaps most simply defined as a representation of a real system or process. A *conceptual model* is a hypothesis for how a system or process operates. This hypothesis can be expressed quantitatively as a mathematical model. *Mathematical models* are abstractions that represent processes as equations, physical properties as constants or coefficients in the equations, and measures of state or potential in the system as variables.

Most groundwater models in use today are deterministic mathematical models. *Deterministic models* are based on conservation of mass, momentum, and energy and describe cause and effect relations. The underlying assumption is that given a high degree of understanding of the processes by which stresses on a system produce subsequent responses in that system, the system's response to any set of stresses can be predetermined, even if the magnitude of the new stresses falls outside the range of historically observed stresses.

Deterministic groundwater models generally require the solution of partial differential equations. Exact solutions can often be obtained analytically, but *analytical models* require that the parameters and boundaries be highly idealized. Some deterministic models treat the properties of porous media as lumped parameters (essentially, as a black box), but this precludes the representation of heterogeneous hydraulic properties in the model. Heterogeneity, or variability in aquifer properties, is characteristic of all geologic systems and is now recognized as playing a key role in influencing groundwater flow and solute transport. Thus, it is often preferable to apply distributed-parameter models, which allow the representation of more realistic distributions of system properties. Numerical methods yield approximate solutions to the governing equation (or equations) through the discretization of space and time. Within the discretized problem domain, the variable internal properties, boundaries, and stresses of the system are approximated. Deterministic, distributed-parameter, *numerical models* can relax the rigid idealized conditions of analytical models or lumped-parameter models, and they can therefore be more realistic and flexible for simulating field conditions (if applied properly).

The number and types of equations to be solved are determined by the concepts of the dominant governing processes. The coefficients of the equations are the parameters that are measures of the properties, boundaries, and stresses of the system; the dependent variables of the equations are the measures of the state of the system and are mathematically determined by the solution of the equations. When a numerical algorithm is implemented in a computer code to solve one or more partial differential equations, the resulting computer code can be considered a *generic model*. When the grid dimensions, boundary conditions, and other parameters (such as hydraulic conductivity and storativity), are specified in an application of a generic model to represent a particular geographic area, the resulting computer program is a *site-specific model*. The ability of generic models to solve the governing equations accurately is typically demonstrated by example applications to simplified problems. This does not guarantee a similar level of accuracy when the model is applied to a complex field problem.

If the user of a model is unaware of or ignores the details of the numerical method, including the derivative approximations, the scale of discretization, and the matrix solution techniques, significant errors can be introduced and remain undetected. For example, if the groundwater flow equation is solved iteratively, but the convergence criterion is relatively too coarse, then the numerical solution may converge, but to a poor solution. The inaccuracy of the solution may or may not be reflected in the mass-balance error. The mass-balance error itself may not be readily observed by inexperienced model users. Unrecognized errors in numerical groundwater models are becoming more possible as user-friendly graphic interfaces make it easier for models to be used (and misused). These interfaces effectively place more distance between the modeler and the numerical method that lies at the core of the model.

20.3 Flow and Transport Processes

The process of groundwater flow is generally assumed to be governed by the relations expressed in Darcy's law (see Chapter 2) and the conservation of mass. However, Darcy's law does have limits on its range of applicability, and these limits must be evaluated in any application.

The purpose of a model that simulates solute transport in groundwater is to compute the concentration of a dissolved chemical species in an aquifer at any specified time and place. The theoretical basis for the equation describing solute transport has been well documented in the literature (e.g., Bear, 1979; Domenico and Schwartz, 1990). Reilly et al. (1987) provide a conceptual framework for analyzing and modeling physical solute-transport processes in groundwater. Changes in chemical concentration occur within a dynamic groundwater system primarily due to four distinct processes: (1) advective transport, in which dissolved chemicals are moving with the flowing groundwater; (2) hydrodynamic dispersion, in which molecular and ionic diffusion and small-scale variations in the flow velocity through the porous media cause the paths of dissolved molecules and ions to diverge or spread from the average direction of groundwater flow; (3) fluid sources, where water of one composition is introduced into and mixed with water of a different composition; and (4) reactions, in which some amount of a particular dissolved chemical species may be added to or removed from the groundwater as a result of chemical, biological, and physical reactions in the water or between the water and the solid aquifer materials or other separate liquid phases.

The subsurface environment constitutes a complex, three-dimensional, heterogeneous hydrogeologic setting. This variability strongly influences groundwater flow and transport, and such a reality can be described accurately only through careful hydrogeologic practice in the field. However, regardless of how much data are collected, uncertainty always remains about the properties and boundaries of the groundwater system of interest. Stochastic approaches have resulted in many significant advances in characterizing subsurface heterogeneity and dealing with uncertainty (see Gelhar, 1993).

20.4 Governing Equations

The mathematical equations that describe groundwater flow (see Chapter 3) and transport processes (see Chapters 14 and 15 and the summary in Chapter 2) may be developed from the fundamental principle of conservation of mass of fluid or of solute. Given a representative elementary volume (REV) of porous medium, a general equation for conservation of mass for the volume may be expressed as:

$$\text{rate of mass inflow} - \text{rate of mass outflow} + \text{rate of mass production/consumption} = \text{rate of mass accumulation} \quad (1)$$

This statement of conservation of mass (or continuity equation) may be combined with a mathematical expression of the relevant process to obtain a differential equation that describes flow or transport.

20.4.1 Groundwater Flow Equation

The rate of flow of water through a porous media is related to the properties of the water, the properties of the porous media, and the gradient of the hydraulic head, as represented by Darcy's law, which can be written as:

$$q_i = -K_{ij}\frac{\partial h}{\partial x_j} \quad (2)$$

where q_i is the specific discharge, LT^{-1}; K_{ij} is the hydraulic conductivity of the porous medium (a second-order tensor), LT^{-1}; and h is the hydraulic head, L.

A general form of the equation describing the transient flow of a compressible fluid in a nonhomogeneous anisotropic aquifer may be derived by combining Darcy's law with the continuity equation. A general groundwater flow equation may be written in Cartesian tensor notation as:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_i}\right)=S_S\frac{\partial h}{\partial t}+W^* \tag{3}$$

where S_S is the specific storage, L^{-1}; t is time, T; W^* is the volumetric flux per unit volume (positive for outflow and negative for inflow), T^{-1}; and x_i are the Cartesian coordinates, L. The summation convention of Cartesian tensor analysis is implied in Equations (2) and (3). Equation (3) can generally be applied if isothermal conditions prevail, the porous medium only deforms vertically, the volume of individual grains remains constant during deformation, Darcy's law applies (and gradients of hydraulic head are the only driving force), and fluid properties (density and viscosity) are homogeneous and constant. Aquifer properties can vary spatially, and fluid stresses (W^*) can vary in space and time.

If the aquifer is relatively thin compared to its lateral extent, it may be appropriate to assume that groundwater flow is areally two-dimensional. This allows the three-dimensional flow equation to be reduced to the case of two-dimensional areal flow, for which several additional simplifications are possible. The advantages of reducing the dimensionality of the equation include less stringent data requirements, smaller computer memory requirements, and shorter computer execution times to achieve numerical solutions.

An expression similar to Equation (3) may be derived for the two-dimensional areal flow of a homogeneous fluid in a confined aquifer and written as:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_i}\right)=S\frac{\partial h}{\partial t}+W \tag{4}$$

where T_{ij} is the transmissivity, L^2T^{-1}; and $T_{ij} = K_{ij}\,b$; b is the saturated thickness of the aquifer, L; S is the storage coefficient (dimensionless); and $W = W^*b$ is the volume flux per unit area, LT^{-1}.

When Equation (4) is applied to an unconfined (water-table) aquifer system, it must be assumed that flow is horizontal and equipotential lines are vertical, that the horizontal hydraulic gradient equals the slope of the water table, and that the storage coefficient is equal to the specific yield (S_y) (Anderson and Woessner, 1992). Note that in an unconfined system, the saturated thickness changes as the water-table elevation (or head) changes. Thus, the transmissivity also can change over space and time (that is, $T_{ij} = K_{ij}b$, where $b(x,y,t) = h - h_b$, and h_b is the elevation of the bottom of the aquifer).

The cross-product terms of the hydraulic conductivity tensor drop out when the coordinate axes are aligned with the principal axes of the tensor; that is, $K_{ij} = 0$ when $i \neq j$. Therefore, the only hydraulic conductivity terms with possible nonzero values are K_{xx} and K_{yy}. Under this assumption, Equation (4) may be simplified to:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right)=S\frac{\partial h}{\partial t}+W \tag{5}$$

for two-dimensional flow.

In some field situations, fluid properties such as density and viscosity may vary significantly in space or time. This may occur where water temperature or dissolved-solids concentration changes significantly. When the water properties are heterogeneous and (or) transient, the relations among water levels, hydraulic heads, fluid pressures, and flow velocities are neither simple nor straightforward. In such cases, the flow equation is written and solved in terms of fluid pressures, fluid densities, and the intrinsic permeability of the porous media (see Konikow and Grove, 1977).

20.4.2 Seepage Velocity

The migration and mixing of chemicals dissolved in groundwater will obviously be affected by the velocity of the flowing groundwater. The specific discharge calculated from Equation (2) is sometimes called the Darcy velocity. However, this nomenclature can be misleading because q_i does not actually represent the speed of water movement. Rather, q_i represents a volumetric flux per unit cross-sectional area. Thus, to calculate the actual seepage velocity of groundwater, one must account for the actual cross-sectional area through which flow is occurring, as follows:

$$V_i=\frac{q_i}{\varepsilon}=-\frac{K_{ij}}{\varepsilon}\frac{\partial h}{\partial x_j} \tag{6}$$

where V_i is the seepage velocity (also commonly called average linear velocity or average interstitial velocity), LT^{-1}; and ε is the effective porosity of the porous medium.

20.4.3 Solute Transport Equation

An equation describing the transport and dispersion of a dissolved chemical in flowing groundwater may be derived from the principle of conservation of mass by considering all fluxes into and out of a representative elementary volume (REV), as described by Bear (1979, p. 29). A generalized form of the solute-transport equation is presented by Grove (1976), in which terms are incorporated to represent chemical reactions and solute concentration both in the pore fluid and on the solid surface, as:

$$\frac{\partial(\varepsilon C)}{\partial t}=\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(\varepsilon C V_i\right)-C'W^*+CHEM \tag{7}$$

where *CHEM* equals one or more of the following:

$-\rho_b\dfrac{\partial \overline{C}}{\partial t}$ for linear equilibrium controlled sorption or ion-exchange reactions,

$\displaystyle\sum_{k=1}^{s} R_k$ for s chemical rate-controlled reactions, and (or)

$-\lambda\left(\varepsilon C+\rho_b\overline{C}\right)$ for decay,

and where D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor), L^2T^{-1}, C' is the concentration of the solute in the source or sink fluid, $\overline{C}$ is the concentration of the species adsorbed on the solid (mass of solute/mass of solid), ρ_b is the bulk density of the sediment, ML^{-3}, R_k is the rate of production of the solute in reaction k, $ML^{-3}T^{-1}$, and λ is the decay constant (equal to ln2/half life), T^{-1} (Grove, 1976).

The first term on the right side of Equation (7) represents the change in concentration due to hydrodynamic dispersion. This expression is analogous to Fick's law describing diffusive flux. This Fickian model assumes that the driving force is the concentration gradient and that the dispersive flux occurs in a direction from higher toward lower concentrations. However, this assumption is not always consistent with field observations and is the subject of much ongoing research and field study (see, for example, Gelhar et al., 1992). The coefficient of hydrodynamic dispersion is defined as the sum of mechanical dispersion and molecular diffusion (Bear, 1979). The mechanical dispersion is a function both of the

intrinsic properties of the porous medium (such as heterogeneities in hydraulic conductivity and porosity) and of the fluid flow. Molecular diffusion in a porous medium will differ from that in free water because of the effects of tortuous paths of fluid connectivity in porous media. These relations are commonly expressed as:

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} + D_m \qquad i, j, m, n = 1,2,3 \tag{8}$$

where α_{ijmn} is the dispersivity of the porous medium (a fourth-order tensor), L; V_m and V_n are the components of the flow velocity of the fluid in the m and n directions, respectively, LT^{-1}; D_m is the effective coefficient of molecular diffusion, L^2T^{-1}; and $|V|$ is the magnitude of the velocity vector, LT^{-1}, defined as $|V| = \sqrt{V_x^2 + V_y^2 + V_z^2}$ (Bear, 1979; Domenico and Schwartz, 1990). The dispersivity of an isotropic porous medium can be defined by two constants. These are the longitudinal dispersivity of the medium, α_L, and the transverse dispersivity of the medium, α_T. These are related to the longitudinal and transverse dispersion coefficients by $D_L = \alpha_L|V|$ and $D_T = \alpha_T|V|$. Most documented applications of transport models to groundwater problems have been based on this conventional formulation, even for cases in which the hydraulic conductivity is assumed to be anisotropic (despite the conceptual inconsistency). However, some models (for example, Voss, 1984) incorporate an additional level of complexity by allowing α_L and (or) α_T to vary with direction.

Although conventional theory holds that α_L is generally an intrinsic property of the aquifer, it is found in practice to be dependent on and proportional to the scale of the measurement. Most reported values of α_L fall in a range from 0.01 to 1.0 times the scale of the measurement, although the ratio of α_L to scale of measurement tends to decrease at larger scales (see Anderson, 1984; Gelhar et al., 1992). Field-scale dispersion (commonly called macrodispersion) results from large-scale spatial variations in hydraulic properties. Consequently, the use of relatively large values of dispersivity together with uniform hydraulic properties (K_{ij} and ε) is inappropriate for describing transport in geological systems (Smith and Schwartz, 1980). Part of the scale dependence of dispersivity may be explained as an artifact of the models used, in that a scaling up of dispersivity will occur whenever an (n-1)-dimensional model is calibrated or used to describe an n-dimensional system (Domenico and Robbins, 1984). Furthermore, if a model applied to a system having variable hydraulic conductivity uses mean values and thereby does not explicitly represent the variability, the model calibration will likely yield values for the dispersivity coefficients that are larger than would be measured locally in the field area. Similarly, representing a transient flow field by a mean steady-state flow field, as is commonly done, inherently ignores some of the variability in velocity and must be compensated for by using increased values of dispersivity (primarily transverse dispersivity) (Goode and Konikow, 1990). Overall, the more accurately a model can represent or simulate the true velocity distribution in space and time, the less of a problem will be the uncertainty concerning representation of dispersion processes.

The mathematical solute-transport model requires at least two partial differential equations. One is the equation of flow, from which groundwater flow velocities are obtained, and the second is the solute-transport equation, whose solution gives the chemical concentration in groundwater. If the properties of the water are affected significantly by changes in solute concentration, as in a saltwater intrusion problem, then the flow and transport equations should be solved simultaneously (or at least iteratively). If the properties of the water remain constant, then the flow and transport equations can be decoupled and solved sequentially, which is simpler numerically.

20.5 Numerical Methods To Solve Equations

The partial differential equations describing groundwater flow and transport can be solved mathematically using either analytical solutions or numerical solutions. The advantages of an analytical solution, when it is possible to apply one, are that it usually provides an exact solution to the governing equation and is often relatively simple and efficient to use. Many analytical solutions have been developed for the flow equation; however, most applications are limited to well hydraulics problems involving radial symmetry. The familiar Theis type curve represents the solution of one such analytical model. Analytical solutions are also available to solve the solute-transport equation (e.g., Bear, 1979; Javandel et al., 1984; Wexler, 1992). In general, obtaining the exact analytical solution to the partial differential equation requires that the properties and boundaries of the flow system be highly and perhaps unrealistically idealized. For simulating most field problems, the mathematical benefits of obtaining an exact analytical solution are probably outweighed by the errors introduced by the simplifying assumptions about the complex field environment that are required to apply the analytical approach.

Alternatively, for problems where the simplified analytical models no longer describe the physics of the situation, the partial differential equations can be approximated numerically. In so doing, the continuous variables are replaced with discrete variables that are defined at grid blocks or nodes. Thus, the continuous differential equation, which defines hydraulic head or solute concentration everywhere in the system, is replaced by a finite number of algebraic equations that defines the hydraulic head or concentration at specific points. This system of algebraic equations generally is solved using matrix techniques. This approach constitutes a numerical model.

Two major classes of numerical methods have come to be well accepted for solving the groundwater flow equation. These are the finite-difference methods and the finite-element methods. Each of these two major classes of numerical methods includes a variety of subclasses and implementation alternatives. Comprehensive treatments of the application of these numerical methods to groundwater problems are presented by Remson et al. (1971) and Wang and Anderson (1982). Both of these numerical approaches require that the area of interest be subdivided by a grid into a number of smaller subareas (cells or elements) that are associated with nodal points (either at the centers or peripheries of the subareas).

In addition to finite-difference and finite-element methods, boundary integral equation methods and analytical element methods can also be applied to solve the flow equation (for example, see Haitjema, 1995). Their main advantage is that, for homogeneous regions, they can provide precise solutions without discretization. Thus, if a system's heterogeneity can be adequately represented by using only a few very large elements, the methods can be very efficient in terms of computer time. If heterogeneities are such that a large number of elements are required to describe them adequately, then finite-difference or finite-element methods may be preferable. To date, finite-difference and finite-element methods have been more widely used than other numerical methods in simulating groundwater flow problems.

Finite-difference methods approximate the first derivatives in the partial differential equations as difference quotients (the differences between values of the independent variable at adjacent nodes with respect to the distance between the nodes, and at two successive time levels with respect to the duration of the time-step increment). Finite-element methods use assumed functions of the dependent variable and parameters to evaluate equivalent integral formulations of the partial differential equations. Huyakorn and Pinder (1983) present a comprehensive analysis of the application of finite-element methods to groundwater problems. In both numerical approaches, the discretization of the space and time dimensions allows the continuous boundary-value problem for the solution of the partial differential equation to be reduced to the simultaneous solution of a set of algebraic equations. These equations can then be solved using either iterative or direct matrix methods.

Each approach has advantages and disadvantages, but there are very few groundwater problems for which either is clearly superior. In general, the finite-difference methods are simpler conceptually and mathematically, and are easier to program. They are typically keyed to a relatively simple, rectangular

grid, which also eases data entry. Finite-element methods generally require the use of more sophisticated mathematics but, for some problems, may be more accurate numerically than standard finite-difference methods. A major advantage of the finite-element methods is the flexibility of the finite-element grid, which allows a close spatial approximation of irregular boundaries of the aquifer and (or) of parameter zones within the aquifer when they are considered. However, the construction and specification of an input data set are much more difficult for an irregular finite-element grid than for a regular rectangular finite-difference grid. Thus, the use of a model preprocessor, which includes a mesh generator and a scheme to number the nodes and elements of the mesh and to specify the spatial coordinates of each node, is recommended. Figure 20.1 illustrates a hypothetical aquifer system, which has impermeable boundaries and a well field (Figure 20.1A), which has been discretized using finite-difference (Figure 20.1B) and finite-element (Figure 20.1C) grids. Figures 20.1B and 20.1C illustrate conceptually how their respective grids can be adjusted to use a finer mesh spacing in selected areas of interest. The rectangular finite-difference grid approximates the aquifer boundaries in a stepwise manner, resulting in some nodes or cells outside the aquifer, whereas sides of the triangular elements of the finite-element grid can closely follow the outer boundary using a minimal number of nodes.

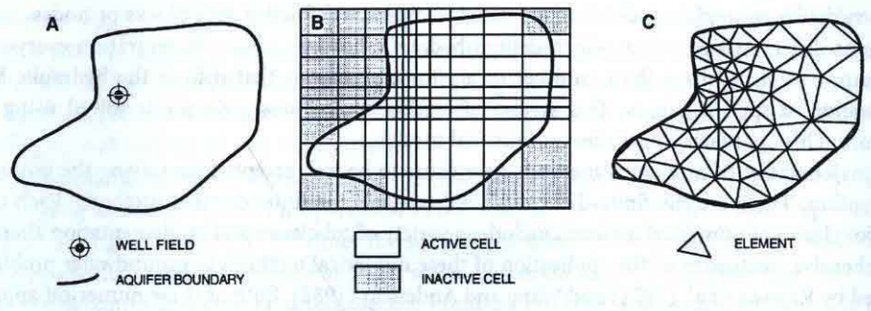

FIGURE 20.1 Hypothetical application to (A) an irregularly bounded aquifer of (B) finite-difference and (C) finite-element grids. (From Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology.* International Atomic Energy Agency, Vienna.)

The solute-transport equation is more difficult to solve numerically than the groundwater flow equation, largely because the mathematical properties of the transport equation vary depending upon which terms in the equation are dominant in a particular situation. When solute transport is dominated by advective transport, as is common in many field problems, then Equation (7) approximates a hyperbolic type of equation (similar to equations describing the propagation of a wave or of a shock front). But if a system is dominated by dispersive fluxes, such as might occur where fluid velocities are relatively low and aquifer dispersivities are relatively high, then Equation (7) becomes more parabolic in nature (similar to the transient groundwater flow equation).

The numerical methods that work best for parabolic partial differential equations are not best for solving hyperbolic equations, and vice versa. Thus, no one numerical method or simulation model will be ideal for the entire spectrum of groundwater transport problems likely to be encountered in the field. Further compounding this difficulty is the fact that in the field, the seepage velocity of groundwater is highly variable, even if aquifer properties are relatively homogeneous because of the effects of complex boundary conditions. Thus, in low permeability zones or near stagnation points, the velocity may be close to zero and the transport processes will be dominated by dispersion processes; in high permeability zones or near stress points (such as pumping wells), the velocity may be several meters per day and the transport processes will be advection dominated. In other words, for the same system, the governing equation may be more hyperbolic in one area (or at one time) and more parabolic in another area (or at another time). Therefore, regardless of which numerical method is chosen as the basis for a simulation model, it will not be ideal or optimal over the entire domain of the problem, and significant numerical

errors may be introduced somewhere in the solution. The transport modeling effort must recognize this inherent difficulty and strive to minimize and control the numerical errors.

Additional complications arise when the solutes of interest are reactive. The reaction terms included in Equation (7) are mathematically simple ones. They do not necessarily represent the true complexities of many reactions. Also, particularly difficult numerical problems arise when reaction terms are highly nonlinear, or if the concentration of the solute of interest is strongly dependent on the concentration of other chemical constituents. In reality, isotherms may not be linear and may not be equilibrium controlled. For field problems in which reactions significantly affect solute concentrations, simulation accuracy is less limited by mathematical constraints than by data constraints. That is, the types and rates of reactions for the specific solutes and minerals in the particular groundwater system of interest are rarely known and require an extensive amount of data to assess accurately.

Finite-difference and finite-element methods also can be applied to solve the transport equation, particularly when dispersive transport is large compared to advective transport. However, numerical errors, such as numerical dispersion and oscillations, may be significant for some problems. The numerical errors can generally be reduced by using a finer discretization (either shorter time steps or finer spatial grid). An example of a documented three-dimensional, transient, finite-difference model that simultaneously solves the fluid pressure, energy-transport, and solute-transport equations for nonhomogeneous miscible fluids is HST3D (Kipp, 1987). An example of a two-dimensional finite-element transport model is SUTRA, documented by Voss (1984).

Although finite-difference and finite-element models are commonly applied to transport problems, other types of numerical methods have also been applied to transport problems, including the method of characteristics, random walk, Eulerian-Lagrangian methods, and adaptive grid methods. All of these methods have the ability to track sharp fronts accurately with a minimum of numerical dispersion. Documented models based on variants of these approaches include Konikow and Bredehoeft (1978), Sanford and Konikow (1985), Prickett et al. (1981), and Zheng (1990).

No single one of the standard numerical methods is ideal for a wide range of transport problems and conditions. Thus, there is currently still much research on developing better mixed or adaptive methods that aim to minimize numerical errors and combine the best features of alternative standard numerical approaches.

20.5.1 Basics of Finite-Difference Methods

The partial differential equations describing the flow and transport processes in groundwater include terms representing derivatives of continuous variables in space and time. Finite-difference methods are based on the approximation of these derivatives (or slopes of curves) by discrete linear changes over discrete intervals of space or time. If the intervals are sufficiently small, then all of the linear increments will represent a good approximation of the true curvilinear surface or hydrograph.

If we consider the observation wells in a confined aquifer, as illustrated in Figure 20.2A, Bennett (1976) shows that a reasonable approximation for the derivative of head, $\partial h/\partial x$, at a point (d) midway between wells 1 and 0 is:

$$\left(\frac{\partial h}{\partial x}\right)_d \approx \frac{h_0 - h_1}{\Delta x} \tag{9}$$

Note that the observation wells are spaced an equal distance apart. Similarly, a reasonable approximation for the second derivative, $\partial^2 h/\partial x^2$, at point 0 (the location of the center well) can be given as:

$$\left(\frac{\partial^2 h}{\partial x^2}\right)_0 \approx \frac{\left(\frac{\partial h}{\partial x}\right)_e - \left(\frac{\partial h}{\partial x}\right)_d}{\Delta x} \approx \frac{\frac{h_2 - h_0}{\Delta x} - \frac{h_0 - h_1}{\Delta x}}{\Delta x} = \frac{h_1 + h_2 - 2h_0}{(\Delta x)^2} \tag{10}$$

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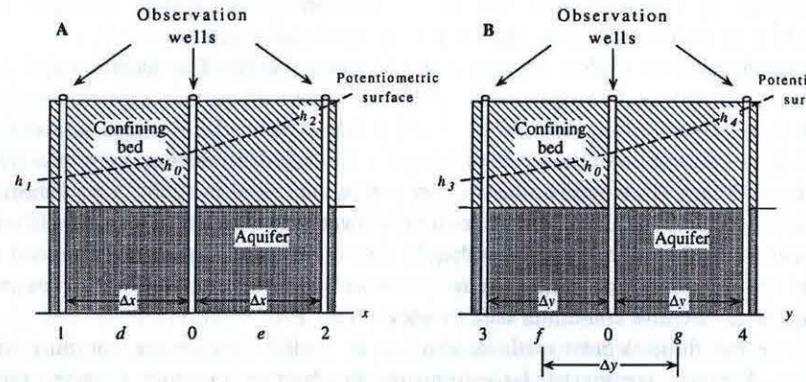

FIGURE 20.2 Schematic cross section through confined aquifer to illustrate numerical approximation to derivatives of head, (A) ∂h/∂x and (B) ∂h/∂y. (Adapted from Bennett, G. D. 1976. *Introduction to Ground-Water Hydraulics: A Programmed Text for Self-Instruction.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 3, Ch. B2.)

If we also consider wells 3 and 4 shown in Figure 20.2B, located on a line parallel to the y-axis, we can similarly approximate $\partial^2 h/\partial y^2$ at point 0 (the same point 0 as in Figure 20.2A) as (Bennett, 1976):

$$\left(\frac{\partial^2 h}{\partial y^2}\right)_0 \approx \frac{h_3 + h_4 - 2h_0}{(\Delta y)^2} \tag{11}$$

If the spacing of the wells in Figure 20.2B is uniform (that is, $\Delta x = \Delta y = a$), then we can develop the following approximation:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \approx \frac{h_1 + h_2 + h_3 + h_4 - 4h_0}{a^2} \tag{12}$$

These approximations can also be obtained through the use of Taylor series expansions. A certain error is involved in approximating the derivatives by finite-differences, but this error will generally decrease as a (or Δx and Δy) is given smaller and smaller values. This error is called a "truncation error" because the replacement of a derivative by a difference quotient is equivalent to using a truncated Taylor series, so that the exact solution of a difference equation differs from the solution of the corresponding differential equation (Peaceman, 1977). Also, it may not be possible to achieve an "exact" solution of the difference equation because of limits of precision in storing numbers in a digital computer. In solving a large set of difference equations, many arithmetic operations are performed, and round-off errors may sometimes accumulate.

Next consider the construction of a rectangular finite-difference grid. Two possible modes of grid construction are illustrated in two dimensions in Figures 20.3A and 3B. In Figure 20.3A, the calculation points (or nodes) are located at the centers of the blocks (or cells) formed by the grid lines. This type of grid is commonly called a block-centered grid. In the second type (Figure 20.3B), the nodes are considered to be located at the intersections of the grid lines. This type has been variously called a point-centered, node-centered, mesh-centered, or lattice-centered grid. Although there is no overall inherent advantage of one type over the other, there will be some operational differences between the two approaches in the treatment of boundaries and in areas of influence around nodes. Most, but not all, finite-difference groundwater models are based on the use of block-centered grids. Double indexing is normally used to identify functions and variables within the two-dimensional region. For example, $h_{i,j}$

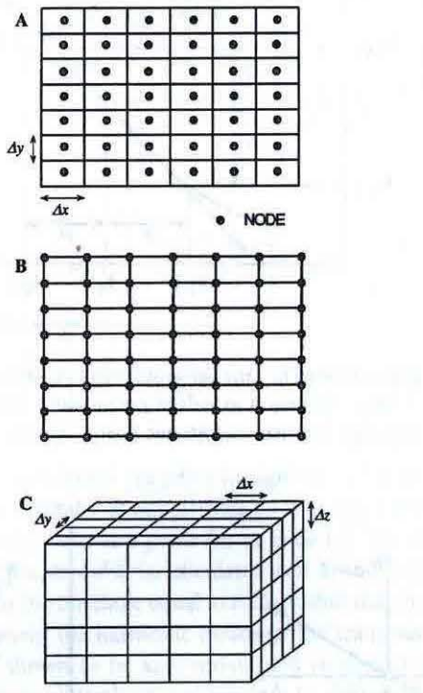

FIGURE 20.3 Examples of finite-difference grids: (A) two-dimensional block-centered grid, (B) two-dimensional node-centered grid, and (C) three-dimensional block-centered grid. (A and B from Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology.* International Atomic Energy Agency, Vienna. C from Konikow, L. F., Goode, D. J., and Hornberger, G. Z. 1996. A three-dimensional method-of-characteristics solute-transport model (MOC3D). U.S. Geol. Survey Water-Res. Inv. Rept. 96-4267).

is the head at node i,j, where i and j are the row and column locations in the finite-difference grid. This procedure is easily extended to three dimensions, as illustrated in Figure 20.3C. Here the vertical dimension (or z-direction) is indexed by the subscript k and $h_{i,j,k}$ would represent the head at node i,j,k.

We must also consider the discretization of time, which may be viewed as another dimension, and hence represented by another index. If we consider a representative segment of a hydrograph (see Figure 20.4), in which head is plotted against time for a transient flow system, n is the index or subscript used to denote the time at which a given head value is observed. The slope of the hydrograph at any point is the derivative of head with respect to time, and it can be approximated as $\partial h/\partial t = \Delta h/\Delta t$. In terms of the heads calculated at specific time increments (or time nodes), the slope of the hydrograph at time n can be approximated by:

$$\left(\frac{\partial h}{\partial t}\right)_{n\Delta t} \approx \frac{h_{n+1} - h_n}{\Delta t} \tag{13}$$

or

$$\left(\frac{\partial h}{\partial t}\right)_{n\Delta t} \approx \frac{h_n - h_{n-1}}{\Delta t} \tag{14}$$

We are calculating the derivative at $t = n\Delta t$ in Equation (13) by taking a "forward difference" from time n to time $n+1$, and by taking a "backward difference" in Equation (14). In terms of solving the

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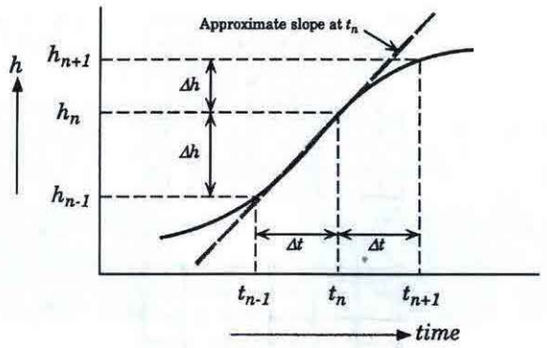

FIGURE 20.4 Part of a hydrograph showing that the derivative (or slope, ∂h/∂t) at time node t_n may be approximated by Δh/Δt. (From Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology.* International Atomic Energy Agency, Vienna.)

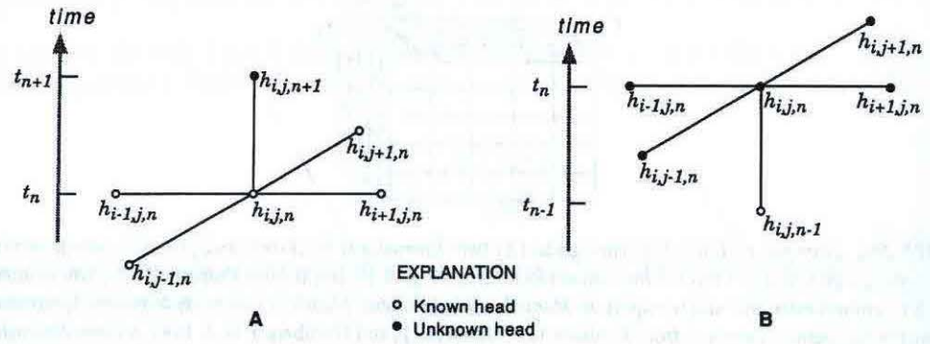

FIGURE 20.5 Grid stencil showing discretization of time at node (i,j) in two-dimensional finite-difference grid: (A) explicit (forward-difference) formulation and (B) implicit (backward-difference) formulation. (From Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology.* International Atomic Energy Agency, Vienna.)

groundwater flow equation for a node (*i,j*) of a finite-difference grid, we have to consider heads at five nodes and at two time levels, as illustrated in Figure 20.5. In Figure 20.5A, we have expressed the spatial derivatives of head at time level n, where all values are known, and the time derivative as a forward difference to the unknown head at time step n+1. Then for every node of the grid we will have a separate difference equation, each of which contains only one unknown variable. Thus, these equations can be solved explicitly. Explicit finite-difference equations are thus simple and straightforward to solve, but they may have associated stability criteria. That is, if time increments are too large, small numerical errors or perturbations may propagate into larger errors at later stages of the computations.

In Figure 20.5B, we have expressed the time derivative as a backward difference from the heads at time level n, which are thereby the unknown heads, whereas the heads at the previous time level, n-1, are known (either from specified initial conditions for the first time step or from subsequent solutions at later time steps). The spatial derivatives of head are written at time level n, where all values are unknown, so for every node of the grid we will have one difference equation that contains five unknowns, which cannot be solved directly. However, for the entire grid, which contains N nodes, we would have a system of N equations containing a total of N unknowns. Such a system of simultaneous equations, together with specified boundary conditions, can be solved implicitly. Although implicit solutions are more complicated, they also have the advantage of generally being unconditionally stable. This implies that a solution will be obtained, although not necessarily that the estimate of the derivative that is calculated

will be accurate, if the time steps are large relative to the rate of change of head. Most available groundwater flow models solve an implicit finite-difference approximation to the flow equation.

We may next consider a two-dimensional groundwater flow equation for a heterogeneous, anisotropic aquifer (Equation [5]), in which the coordinate system is aligned with the major axes of the transmissivity tensor. This may be approximated by the following finite-difference equation for representative node (*i,j*) as:

$$T_{xx[i-\frac{1}{2},j]}\left(\frac{h_{i-1,j,n}-h_{i,j,n}}{(\Delta x)^2}\right)+T_{xx[i+\frac{1}{2},j]}\left(\frac{h_{i+1,j,n}-h_{i,j,n}}{(\Delta x)^2}\right)+T_{yy[i,j-\frac{1}{2}]}\left(\frac{h_{i,j-1,n}-h_{i,j,n}}{(\Delta y)^2}\right)$$
$$+T_{yy[i,j+\frac{1}{2}]}\left(\frac{h_{i,j+1,n}-h_{i,j,n}}{(\Delta y)^2}\right)=S\left(\frac{h_{i,j,n}-h_{i,j,n-1}}{\Delta t}\right)-\frac{q_{i,j}}{\Delta x\Delta y}-\frac{K_z}{m}\left(H_{s[i,j]}-h_{i,j,n}\right) \quad (15)$$

where $q_{i,j}$ is the volumetric rate of withdrawal (negative in sign) or recharge (positive) at the i,j node, L^3T^{-1}. This formulation inherently assumes that any stresses, such as represented by $q_{i,j}$, are applied over the entire surface area of cell i,j rather than at a point (or at node i,j). This implies that if a pumping well is represented at node i,j, then the head will be calculated as if it were being withdrawn from a well that had a horizontal surface area for the borehole equal to ΔxΔy rather than its actual value. In Equation (15), the transmissivity terms represent the harmonic means of the transmissivity of the two adjacent cells. The harmonic mean can be shown to be appropriate and consistent with the assumption that transmissivity is constant and uniform within each cell but may be different between cells. Other types of means for interblock transmissivity may be more appropriate for other assumptions about the transmissivity distribution, such as smoothly varying transmissivity (Goode and Appel, 1992).

20.5.2 Basics of Finite-Element Methods

The finite-element method (FEM) is a numerical analysis technique for obtaining approximate solutions to a wide variety of problems in physics and engineering. The method was originally applied to structural mechanics but is now used in all fields of continuum mechanics. Huebner (1975) describes four different approaches to formulate the finite-element method for a problem, which are: the direct approach, the variational approach, the weighted residual approach, and the energy balance approach. In groundwater problems, the approach frequently used is either the weighted residual or variational approach.

The finite-element method (FEM) uses a concept of "piecewise approximation." The domain of the problem, that is the extent of the aquifer to be simulated, is divided into a set of elements or pieces. In theory, the elements can be of different shapes and sizes. Most FEM computer programs use one shape element, most commonly either triangular or quadrilateral elements. In the groundwater model MODFE (Torak, 1993; Cooley, 1992) triangular elements are used, whereas in the groundwater model SUTRA (Voss, 1984) quadrilateral elements are used. Point values of the dependent variable (for example, head, pressure, or concentration) are calculated at nodes, which are the corners or vertices of the elements, and a simple equation is used to describe the value of the dependent variable within the element. This simple equation is called a basis function and each node that is part of an element has an associated basis function. The simplest basis functions that are usually used are linear functions. The solution to the differential equation for flow (Equation [3]) or transport (Equation [7]) is approximated by a set of elements in which the dependent variable only varies linearly within the element, but the entire set of elements approximates the complex distribution of head or concentration. Figure 20.6 shows the approximate modeled hydraulic head distribution (Figure 20.6C) comprised of a set of triangular elements (Figure 20.6A) having a linear approximation of head variation within each element (Figure 20.6B).

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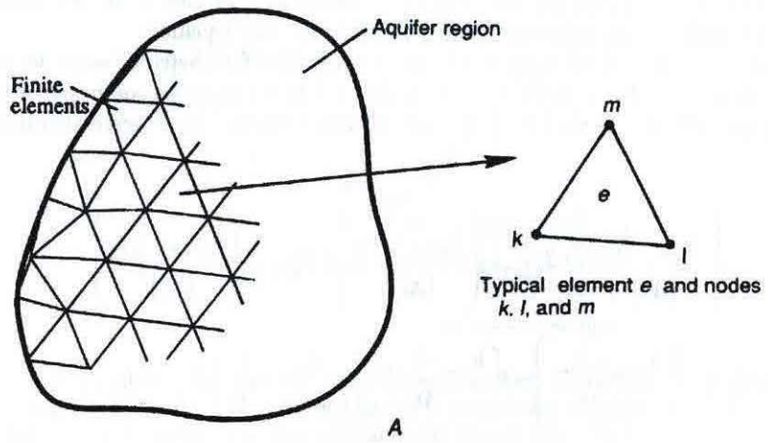

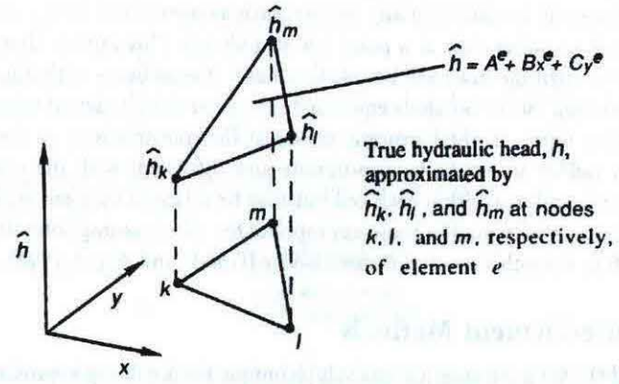

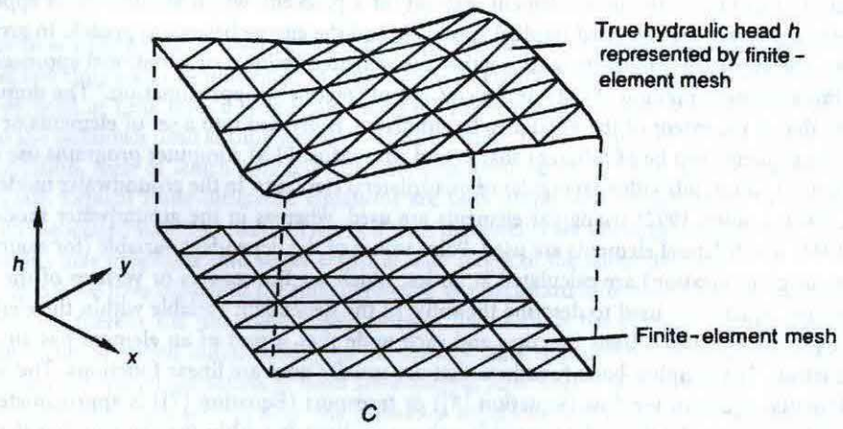

FIGURE 20.6 Diagram showing (A) aquifer region partially subdivided by finite elements and typical element e, (B) finite-element representation of hydraulic head $\hat{h}$, and (C) finite-element mesh configuration for approximating true hydraulic head. (From Torak, L. J. 1993. A modular finite-element model (MODFE) for areal and axisymmetric ground-water-flow problems, Part 1: Model description and user's manual. Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 6, Ch. A3.)

In the method of weighted residuals, the piecewise continuous surface is obtained by minimizing the difference between the approximate surface and the continuous surface. The method of weighted residuals is summarized by Huyakorn and Pinder (1983, p. 39) as follows. Any differential equation L(h), such as the steady-state form of Equation (3) (the groundwater flow equation) can be written:

$$L(h) = 0 \tag{16}$$

over the domain of the problem *R*. The first step in obtaining the approximate solution is to define the approximate solution as the sum of all the simple basis functions as:

$$\hat{h} = \sum_{i=1}^{n} N_i Z_i \tag{17}$$

where $\hat{h}$ is the approximate solution, n is the number of linearly independent basis functions, N_i are the linearly independent basis functions defined over the entire domain, and Z_i are the unknown coefficients to be determined (there is one coefficient for each node in the finite-element mesh). The trial function $\hat{h}$ is an approximation, so that when it is substituted into Equation (16) there will be some error, ξ, defined as:

$$\xi = L(\hat{h}) \tag{18}$$

The method of weighted residuals determines the unknown coefficients by minimizing the error. This is accomplished by weighting the error, integrating the error, and setting the error equal to zero over the entire domain. A weighting function, W_i, can be specified for each basis function and the resulting integration is:

$$\int_R W_i \xi \, dR = \int_R W_i L(\hat{h}) \, dR = 0 \qquad i = 1,2 \ldots n \tag{19}$$

Equation (17) is substituted into Equation (19), and weighting functions are specified. There are then n equations and n unknowns. The selection of the weighting functions and the simplification of the integral in Equation (19) into a linear algebraic equation is mathematically straightforward, but not intuitive. In the Galerkin method, the weighting functions are chosen to be identical to the basis functions, and Equation (19) is simplified by using integration by parts. Because the basis functions and weighting functions are defined to be of a specific algebraic form (for example, linear basis functions), the modified integral is straightforward to solve and becomes a set of n simultaneous algebraic equations.

After Equation (19) is mathematically evaluated into a set of n simultaneous equations, they are solved using matrix solution techniques for the n unknown coefficients Z_i, and the approximate solution $\hat{h}$ is determined at each node. The time derivative is frequently approximated by finite differences as discussed in the previous section. Huyakorn and Pinder (1983), Huebner (1975), Zienkiewicz (1971), Wang and Anderson (1982), and Cooley (1992) provide more comprehensive explanations of the method.

20.5.3 Basics of Method-of-Characteristics Methods

The method of characteristics was developed to solve hyperbolic differential equations (advectively dominated transport equations). A major advantage is that the method minimizes numerical dispersion

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(Reddell and Sunada, 1970; Garder et al., 1964; Zheng and Bennett, 1995). The approach taken by the method of characteristics is not to solve Equation (7) directly, but rather to solve an equivalent system of ordinary differential equations. A form of Equation (7), accounting for equilibrium-controlled sorption or exchange and first-order irreversible rate reactions, can be further modified for improved compatibility with this method by expanding the advection term, substituting relations from Darcy's law and the flow equation, and rearranging terms to obtain:

$$\frac{\partial C}{\partial t} = \frac{1}{R_f}\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{V_i}{R_f}\frac{\partial C}{\partial x_i} + \frac{W^*\left(C - C'\right)}{\varepsilon R_f} - \lambda C \tag{20}$$

where R_f is defined as a dimensionless retardation factor, $R_f = 1 + \frac{\rho_b K_d}{\varepsilon}$, and K_d is the distribution coefficient, L^3M^{-1}. If we consider the material derivative of concentration with respect to time, dC/dt, as describing the change in concentration of a parcel of water moving at the seepage velocity of water, it may be defined for a two-dimensional system as:

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + \frac{\partial C}{\partial x}\frac{dx}{dt} + \frac{\partial C}{\partial y}\frac{dy}{dt} \tag{21}$$

The second and third terms on the right side include the material derivatives of position, which are defined by the velocity in the x and y directions. We then have:

$$\frac{dx}{dt} = \frac{V_x}{R_f} \tag{22}$$

$$\frac{dy}{dt} = \frac{V_y}{R_f} \tag{23}$$

and

$$\frac{dC}{dt} = \frac{1}{R_f}\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) + \frac{W^*\left(C - C'\right)}{\varepsilon R_f} - \lambda C \tag{24}$$

The solutions of the system of equations comprising Equations (22) through (24) may be given as $x = x(t)$, $y = y(t)$, and $C = C(t)$, and are called the characteristic curves of Equation (20). Given solutions to Equations (22) through (24), a solution to the partial differential equation may be obtained by following the characteristic curves, which are defined by the particle pathlines. This may be accomplished by introducing a set of moving points (or reference particles) that can be traced within the stationary coordinates of a finite-difference grid. Each particle corresponds to one characteristic curve, and values of x, y, and C are obtained as functions of t for each characteristic (Garder et al., 1964). Each point has a concentration and position associated with it and is moved through the flow field in proportion to the flow velocity at its location (see Figure 20.7). The concentrations at the nodes of the fixed finite-difference grid may then be estimated as an arithmetic or weighted mean of the concentrations of all particles contained within the cell area for that node.

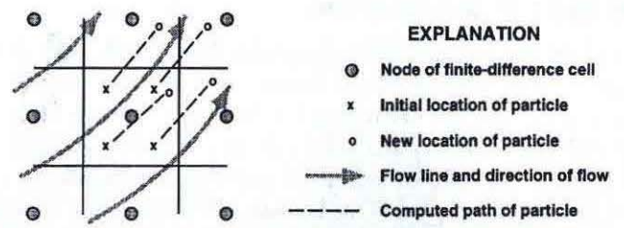

FIGURE 20.7 Part of a hypothetical finite-difference grid showing relation of flow field to movement of points (or particles) in method-of-characteristics model for simulating solute transport. (Adapted from Konikow, L. F. and Bredehoeft, J. D. 1978. *Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 7, Ch. C2.)

20.5.4 Matrix Solution Techniques

As indicated, the finite-difference and finite-element approximations lead to an algebraic equation for each node point. The set of algebraic equations may be solved numerically by one of two basic methods: direct or iterative. In direct methods, a sequence of operations is performed only once to solve the matrix equation, providing a solution that is exact, except for machine round-off error. Iterative methods arrive at a solution by a process of successive approximation. They involve making an initial guess at the solution, then improving this guess by some iterative process until an error criterion is satisfied. Therefore, in these techniques, convergence and the rate of convergence are of concern.

Direct methods can be further subdivided into: (1) solution by determinants, (2) solution by successive elimination of the unknowns, and (3) solution by matrix inversion. Direct methods have two main disadvantages. The first problem is one of computer resource requirements, including large storage (memory) requirements and long computation times for large problems. The matrix is sparse (contains many zero values) and to minimize computational effort, several techniques have been proposed. However, for finite-difference and finite-element methods, storage requirements may still prove to be unavoidably large for three-dimensional problems. The second problem with direct methods is round-off error. Because many arithmetic operations are performed, round-off errors can accumulate for certain types of matrices.

Iterative schemes avoid the need for storing large matrices, which make them attractive for solving problems with many unknowns. Numerous schemes have been developed; a few of the more commonly used ones include successive over-relaxation methods, iterative alternating-direction implicit procedure, and the strongly implicit procedure.

Because iterative methods start with an initial estimate for the solution, the efficiency of the method depends somewhat on this initial guess. To speed up the iterative process, relaxation and acceleration factors are used. Unfortunately, the definition of best values for these factors commonly is problem dependent. In addition, iterative approaches require that an error tolerance be specified to stop the iterative process. An optimal value for the tolerance, which is used to evaluate when the iterative calculations have converged on a solution, may also be problem dependent. If the tolerance is set too large, then the iterations may stop before adequate numerical accuracy is achieved. If the tolerance is set too small, then the iterative process may consume excessive computational resources in striving for numerical precision that may be orders of magnitude smaller than the precision of the field data, or the iterative process may even fail to converge.

More recently, a semi-iterative method, or class of methods, known as conjugate-gradient methods, has gained popularity. One advantage of the conjugate-gradient method is that it does not require the use or specification of iteration parameters, thereby eliminating this partly subjective procedure.

20.5.5 Boundary and Initial Conditions

To obtain a unique solution of a partial differential equation corresponding to a given physical process, additional information about the physical state of the process is required. This information is supplied by boundary and initial conditions. For steady-state problems, only boundary conditions are required, whereas for transient problems, boundary and initial conditions must be specified.

Mathematically, the boundary conditions include the geometry of the boundary and the values of the dependent variable or its derivative normal to the boundary. In physical terms, for groundwater model applications, the boundary conditions are generally of three types: (1) specified value (head or concentration), (2) specified flux (corresponding to a specified gradient of head or concentration), or (3) value-dependent flux (or mixed boundary condition, in which the flux across a boundary is related to both the normal derivative and the value) (Mercer and Faust, 1981; Franke et al., 1987). The third type of boundary condition might be used, for example, to represent leakage or exchange between a stream and an adjacent aquifer, in which the leakage may change over time as the head in the aquifer changes, even though the head in the stream might remain fixed. A no-flow boundary is a special case of the second type of boundary condition. The types of boundaries appropriate to a particular field problem require careful consideration.

The initial conditions are simply the values of the dependent variable specified everywhere inside the boundary at the start of the simulation. Normally, the initial conditions are specified to be a steady-state solution. If, however, initial conditions are specified so that transient flow is occurring in the system at the start of the simulation, it should be recognized that heads will change during the simulation, not only in response to the new pumping stress, but also due to the initial conditions (Franke et al., 1987).

20.6 Model Design, Development, and Application

The first step in model design and application is to define the nature of the problem and the purpose of the model. Although this may seem obvious, it is an important first step that is sometimes overlooked in a hasty effort to take action. This step is closely linked with the formulation of a conceptual model, which again is required prior to development of a mathematical model. A possible outcome of such a preliminary assessment might even be that a deterministic simulation model is not needed. In formulating a conceptual model, the analyst must evaluate which processes are significant in the system being investigated for the particular problem at hand. Some processes may be important to consider at one scale of study, but negligible or irrelevant at another scale of investigation. The analyst must similarly decide on the appropriate dimensionality for the numerical model. Good judgment is required to evaluate and balance the trade-offs between accuracy and cost, with respect to model development, model use, and data requirements. The key to efficiency and accuracy in modeling a system probably is more affected by the formulation of a proper and appropriate conceptual model than by the choice of a particular numerical method or code.

Once a decision to develop a model has been made, a code (or generic model) must be selected (or modified or constructed) that is appropriate for the given problem. Next, the generic code must be adapted to the specific site or region being simulated. Development of a numerical deterministic, distributed-parameter, simulation model involves selecting or designing spatial grids and time increments that will yield an accurate solution for the given system and problem. The analyst must then specify the properties of the system (and their distributions), stresses on the system (such as recharge and pumping rates), boundary conditions, initial conditions (for transient problems), and geochemical processes/reactions (if appropriate). All of the parameter specifications and boundary conditions are really part of the overall conceptual model of the system, and the initial numerical model reflects the analyst's conceptual model of the system.

It must always be remembered that a model is an approximation of a very complex reality, and a model is used to simplify that reality in a manner that captures or represents the essential features and processes relative to the problem at hand. In the development of a deterministic groundwater model for a specific

area and purpose, an appropriate level of model complexity (or, rather, simplicity) must be selected. One may be inclined to believe that finer resolution in a model will yield greater accuracy, and there is a legitimate basis for this. However, there also exists the practical constraint that even when appropriate data are available, a finely discretized three-dimensional numerical model may be too large to run on available computers, especially if transport processes are included. The selection of the appropriate model and appropriate level of model complexity remains subjective and dependent on the judgment and experience of the analysts, the objectives of the study, the level of prior information available for the system of interest, and the complexity of the system being modeled. The trade-off between model accuracy and model cost will always be a difficult one to resolve, but will always have to be made. In any case, water managers and other users of model results must be made aware that these trade-offs and judgments have been made and may affect the reliability of the model.

In general, it is more difficult to calibrate a solute-transport model of an aquifer than it is to calibrate a groundwater flow model. Fewer parameters need to be defined to compute the head distribution with a flow model than are required to compute concentration changes with similar confidence using a solute-transport model. Also, in typical field problems, defining the source term for a solute-transport model is especially difficult for point-source contamination problems because the timing and strength of releases of solute mass into an aquifer system are rarely known or reported accurately (and, in fact, are commonly the very point of contention in litigation).

Because the groundwater seepage velocity is determined from the head distribution, and because both advective transport and hydrodynamic dispersion are functions of the seepage velocity, a model of groundwater flow is typically calibrated before a solute-transport model is developed. In fact, in a field environment perhaps the single most important key to understanding a solute-transport problem is the development of an accurate definition (or model) of the flow system. This is particularly relevant to transport in fractured rocks, where simulation is commonly based on porous-media concepts. In highly heterogeneous systems, the potential (or head) field can often be simulated fairly accurately, whereas the calculated velocity field may still be greatly in error, resulting in considerable errors in simulations of transport.

20.6.1 Generic Model Verification

One of the first things that must be demonstrated is that the generic model accurately solves the governing equations for various boundary value problems, an evaluation that is often called model "verification." This is checked by demonstrating that the code gives good results for problems having known solutions. This test is usually done by comparing the numerical model results to that of an analytical solution. Numerical accuracy is rarely a problem for the solution to the flow equation, but may sometimes be a significant problem in transport modeling.

It must be remembered that numerical solutions are sensitive to spatial and temporal discretization. Therefore, even a perfect agreement for test cases only proves that the numerical code can accurately solve the governing equations, not that it will accurately solve problems under any and all circumstances.

Analytical solutions generally require simple geometry, uniform properties, and idealized boundary and initial conditions. The power of the numerical methods is that they are not constrained by the simplification imposed by analytical methods and allow the introduction of nonhomogeneous, anisotropic parameter sets, irregular geometry, mixed boundary conditions, and even nonlinearities into the boundary value problems. Usually, analytical solutions approximating these complexities are unavailable for comparison. Therefore, once these complexities are introduced there is no definitive basis for verifying the numerical model.

One approach that improves confidence for complex heterogeneous problems is to compare the model results to experimental data, to results of other well-accepted models, or to some other accepted standard. Such evaluations might best be termed benchmarking. The HYDROCOIN Project used standardized problem definitions as a basis for intercode comparisons (Swedish Nuclear Power Inspectorate, 1987). While this type of benchmarking helps assure consistency, it does not guarantee or measure accuracy. A

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collection and detailed discussion of a number of classical groundwater problems that have been used historically as a basis of model evaluation are presented and documented by Ségol (1994).

20.6.2 Grid Design

The dimensionality of the model (i.e., one, two, or three dimensions) should be selected during the formulation of the conceptual model. If a one- or two-dimensional model is selected, then it is important that the grid be aligned with the flow system so that there is no unaccounted flux into or out of the line or plane of the grid. For example, if a two-dimensional areal model is applied, then there should be no significant vertical components of flow and any vertical leakage or flux must be accounted for by boundary conditions; if a two-dimensional profile model is applied, then the line of the cross section should be aligned with an areal streamline, and there should not be any significant lateral flow into or out of the plane of the cross section.

To minimize a variety of sources of numerical errors, the model grid should be designed using the finest mesh spacing and time steps that are possible, given limitations on computer memory and computational time. To the extent possible, the grid should be aligned with the fabric of the rock and with the average direction of groundwater flow. The boundaries of the grid also should be aligned, to the extent possible, with natural hydrologic and geologic boundaries of the system of interest. Where it is impractical to extend the grid to a natural boundary, then an appropriate boundary condition should be imposed at the edge of the grid to represent the net effects of the continuation of the system beyond the grid. This can typically be accomplished using head-dependent leakage (third type) boundary conditions. However, this would preclude calculating (and accounting for) any storage changes outside the active grid. These boundaries should also be placed as far as possible away from the area of interest and areas of stresses on the system, so as to minimize any impact of conceptual errors associated with these artificial boundary conditions. Note that it is possible for certain types of hydraulic boundaries, such as a groundwater divide, to change location over time if they are located near a major hydraulic stress. If this is anticipated, it might be preferable to extend the boundary of the grid some distance beyond the location of such a natural boundary.

In designing the grid, the length-to-width ratio (or aspect ratio) of cells or elements should be kept as close to one as possible. Long linear cells or elements can lead to numerical instabilities or errors, and should be avoided, particularly if the aspect ratio is greater than about five (Bear and Verruijt, 1987). However, this is a loose guideline as aspect ratios exceeding 100:1 are often used without introducing significant error. In applying this guideline to triangular finite-element methods, Torak (1993) recommends that angles less than 22.5° in a triangle should be avoided.

In specifying boundary conditions for a particular problem and grid design, care must be taken not to overconstrain the solution. That is, if dependent values are fixed at too many boundary nodes, at either internal or external nodes of a grid, the model may have too little freedom to calculate a meaningful solution. At the extreme, by manipulating boundary conditions, one can force any desired solution at any given node. While a forced solution may assure a perfect match to observed data used for calibration, such a match is, of course, not an indicator of model accuracy or reliability and, in fact, can be meaningless (Franke and Reilly, 1987).

To optimize computational resources in a model, it is sometimes advisable to use an irregular (or variably spaced) mesh in which the grid is finest in areas of point stresses, where gradients are steepest, where data are most dense, where the problem is most critical, and (or) where greatest numerical accuracy is desired. It is generally advisable to increase the mesh spacing by a factor no greater than about two between adjacent cells or elements. Similarly, time steps can often be increased geometrically during a transient simulation. At the initial times or after a change in the stress regime, very small time steps should be imposed, because that is when changes in the dependent variable over time are the greatest. As elapsed time increases, the rate of change in head typically decreases, so time steps can often be safely increased by a factor of two or more.

Because transmissivity is a property of the porous media, the cross-product terms of the transmissivity tensor drop out of the governing flow equation that is solved in a model by aligning the model grid with the major axes of the transmissivity tensor (as represented in Equation [5]). This makes the code simpler and more efficient, and, in fact, is a required assumption for most finite-difference models. However, this same simplification typically is not possible for the dispersion tensor in the transport equation because it is also related to, and depends on, the flow direction, which changes orientation over space and time. In general, it is not possible to design a fixed grid that will always be aligned with a changing flow field.

20.6.3 Model Calibration

Deterministic groundwater simulation models impose large requirements for data to define all of the parameters at all of the nodes of a grid. To determine uniquely the parameter distribution for a field problem, so much expensive field testing would be required that it is seldom feasible either economically or technically. Therefore, the model typically represents an attempt, in effect, to solve a large set of simultaneous equations having more unknowns than equations. It is inherently impossible to obtain a unique solution to such a problem.

Uncertainty in parameters logically leads to a lack of confidence in the interpretations and predictions that are based on a model analysis, unless the model can be demonstrated to be a reasonably accurate representation of the real system. To demonstrate that a deterministic groundwater simulation model is realistic, usually field observations of aquifer responses (such as changes in water levels for flow problems or changes in concentration for transport problems) are compared to corresponding values calculated by the model. The objective of this calibration procedure is to minimize differences between the observed data and calculated values. Usually, the model is considered calibrated when it reproduces historical data within some acceptable level of accuracy. The level of acceptability is, of course, determined subjectively. Although a poor match provides evidence of errors in the model, a good match in itself does not prove the validity or adequacy of the model (Konikow and Bredehoeft, 1992).

Because of the large number of variables in the set of simultaneous equations represented in a model, calibration will not yield a unique set of parameters. Where the match is poor, it suggests (1) an error in the conceptual model, (2) an error in the numerical solution, or (3) a poor set of parameter values. Even when the match to historical data is good, the model may still fail to predict future responses accurately, especially under a newer or more extended set of stresses than were experienced during the calibration period.

The calibration of a deterministic groundwater model is often accomplished through a trial and error adjustment of the model's input data (aquifer properties, sources and sinks, and boundary and initial conditions) to modify the model's output. Because a large number of interrelated factors affect the output, trial and error adjustment may become a highly subjective and inefficient procedure. Advances in parameter estimation procedures help to eliminate some of the subjectivity inherent in model calibration (Yeh, 1986). The newer approaches generally treat model calibration as a statistical procedure using multiple regression approaches. Parameter estimation procedures allow the simultaneous construction, application, and calibration of a model using uncertain data, so that the uncertainties in model parameters and in predictions and assessments can be quantified.

However, even with regression modeling, the hydrologic experience and judgment of the modeler continues to be a major factor in calibrating a model both accurately and efficiently. In any case, the modeler should be very familiar with the specific field area being studied in order to ensure that both the data base and the numerical model adequately represent prevailing field conditions. The modeler must also recognize that uncertainty in specification of sources, sinks, and boundary and initial conditions should be evaluated during the calibration procedure in the same manner as uncertainty in aquifer properties. Failure to recognize the uncertainty inherent both in the input data and in the calibration data may lead to "fine-tuning" of the model through unjustifiably precise parameter adjustments strictly to improve the match between observed and calculated variables. This may serve only to provide a false

confidence in the model without producing an equivalent (or any) increase in the predictive accuracy of the model or any improved conceptual understanding of the real system. Freyberg (1988) illustrated this in an exercise in which several groups were given the task of modeling a particular hypothetical groundwater problem. The group that achieved the best calibration, as measured by the minimum root mean square error, was not the group that developed the model that yielded the best prediction (measured by the same criterion). Freyberg (1988, p. 360) concluded that "simple measures of the goodness of a calibrated fit to head data are inadequate to evaluate the true worth of a calibrated parameter set."

Figure 20.8 illustrates in a general manner the use and role of deterministic models in the analysis of groundwater problems. The value of the modeling approach is its capability to integrate site-specific data with equations describing the relevant processes as a quantitative basis for predicting changes or responses in a groundwater system. There must be allowances for feedback from the stage of interpreting model output both to the data collection and analysis phase and to the conceptualization and mathematical definition of the relevant governing processes. One objective of model calibration should be to improve the conceptual model of the system. Because the model quantitatively integrates the effects of the many factors that affect groundwater flow or solute transport, the calculated results should be internally consistent with all input data, and it can be determined if any element of the conceptual model should be revised. In fact, prior concepts or interpretations of aquifer parameters or variables, such as represented by potentiometric maps or the specification of boundary conditions, may be revised during the calibration procedure as a result of feedback from the model's output. In a sense, any adjustment of input data constitutes a modification of the conceptual model.

Automated parameter-estimation techniques improve the efficiency of model calibration and have two general components — one part that calculates the best fit (sometimes called automatic history matching) and a second part that evaluates the statistical properties of the fit. The objective of automatic history matching is to obtain the estimates of system parameters that yield the closest match (minimize deviations) between observed data and model calculations. Least squares deviation is usually chosen as a criterion. The minimization procedure uses sensitivity coefficients that are based on the change in calculated value divided by the change in the parameter. For groundwater flow, for example, this may

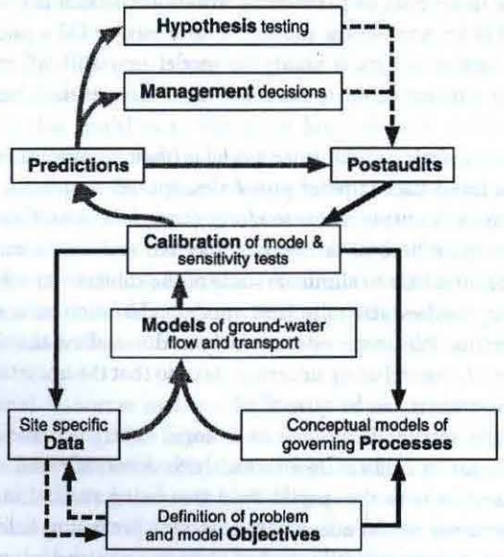

FIGURE 20.8 The use and role of models in the analysis of groundwater problems. (Adapted from Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology*. International Atomic Energy Agency, Vienna.)

take the specific form of $\partial h/\partial T$; that is, the change in head with changing transmissivity. The sensitivity coefficients themselves may be useful in the consideration of additional data collection.

Parameter uncertainty is commonly addressed using a sensitivity analysis. A major objective of sensitivity analysis of simulation models is to determine the change in model results as a result of changes in the model input or system parameters. Conventional sensitivity analysis uses direct parameter sampling in which parameters are perturbed one by one and the complete set of system equations are resolved (Konikow and Mercer, 1988). Sensitivity coefficients for each of these perturbed parameters may be derived by a finite-difference approximation.

20.6.4 Model Error

Discrepancies between observed and calculated responses of a system are the manifestation of errors in the conceptual or mathematical model. In applying groundwater models to field problems, there are three sources of error, and it may not be possible to distinguish among them (Konikow and Bredehoeft, 1992). One source is conceptual errors — that is, misconceptions about the basic processes that are incorporated in the model. Conceptual errors include both neglecting relevant processes as well as inappropriate representation of processes. Examples of such errors include the use of a two-dimensional model where significant flow or transport occurs in the third dimension, or the application of a model based upon Darcy's law to media or environments where Darcy's law is inappropriate. A second source of error involves numerical errors arising in the equation-solving algorithm. These include truncation errors, round-off errors, and numerical dispersion. A third source of error arises from uncertainties and inadequacies in the input data that reflect our inability to describe comprehensively and uniquely the aquifer properties, stresses, and boundaries. In most model applications, conceptualization problems and uncertainty concerning the input data are the most common sources of error.

Numerical methods in general yield approximate solutions to the governing equations. There are a number of possible sources of numerical error in the solution. If model users are aware of the source and nature of these errors, they can control them and interpret the results in light of the presence of error. In solving advection-dominated transport problems in which a relatively sharp front (or steep concentration gradient) is moving through a system, it is numerically difficult to preserve the sharpness of the front.

Obviously, if the width of the front is narrower than the node spacing, then it is inherently impossible to calculate the correct values of concentration in the vicinity of the sharp front. However, even in situations where a front is less sharp, the numerical solution technique can calculate a greater dispersive flux than would occur by physical dispersion alone or would be indicated by an exact solution of the governing equation. That part of the calculated dispersion (or spreading of solute about the center of mass) introduced solely by the numerical solution algorithm is called numerical dispersion.

Figure 20.9 illustrates calculated breakthrough curves for a hypothetical problem of uniform flow and transport to the right, at some time and distance after a tracer having a relative concentration of 1.0 was injected at some point upstream. Curve A represents the breakthrough curve and position of a sharp front for a case having no dispersion (plug flow). Curve B represents an exact analytical solution for a nonzero dispersivity. Curve C illustrates the breakthrough curve calculated for the same conditions as B, but using a numerical method that introduces numerical dispersion. Significant differences exist between the analytical solution (B) and the numerical solution (C) in parts of the domain. Therefore, care must be taken to assess and minimize such numerical errors that would artificially add "numerical" spreading or mixing to the calculated dispersion attributable to physical and chemical processes.

Numerical dispersion can be controlled by reducing the grid spacing (Δx and Δy). However, reduction to a tolerable level may require an excessive number of nodes and render the computational costs unacceptably high. It may also be controlled in finite-element methods by using higher order basis functions or by adjusting the formulation of the equations (using different combinations of forward, backward, or centered in time and/or space, or using different weighting functions). Unfortunately, many approaches that eliminate or minimize numerical dispersion introduce oscillatory behavior, causing

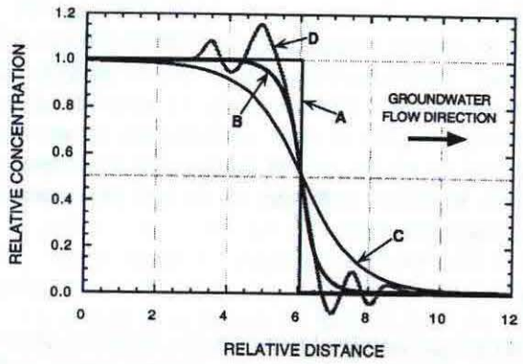

FIGURE 20.9 Representative breakthrough curves for a simple flow and transport problem to illustrate types of numerical errors that may occur in numerical solution to transport equation: (A) plug flow having no dispersion, (B) "exact" solution for transport with dispersion, (C) numerical solution for case B that exhibits effects of numerical dispersion, and (D) numerical solution for case B that exhibits oscillatory behavior. (Adapted from Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology*. International Atomic Energy Agency, Vienna.)

overshoot behind a moving front and possibly undershoot ahead of the front (see curve D in Figure 20.9), and vice versa. Undershoot can result in the calculation of negative concentrations, which are obviously unrealistic. Overshoot can introduce errors of equal magnitude that may go unnoticed because the value is positive in sign (although greater than the source concentration, so still unrealistic). Oscillations generally do not introduce any mass balance errors, and often dampen out over simulation time. However, in some cases, oscillatory behavior can become unbounded, yielding an unstable solution or failure to converge numerically.

In solving the advective-dispersive transport equation, some numerical errors (mainly oscillations) can be related to two dimensionless parameter groups (or numbers). One is the Peclet number, P_e, which may be defined as $P_e = \Delta l/\alpha$, where Δl is a characteristic nodal spacing (although it should be noted that there are several alternative, though essentially equivalent, ways to define P_e). Anderson and Woessner (1992) recommend that the grid be designed so that $\Delta l < 4\alpha$ (or $P_e < 4$); Ségol (1994) recommends a criterion of $P_e \leq 2$. Similarly, time discretization can be related to the Courant number, C_o, which may be defined as $C_o = V\Delta t/\Delta l$ (Anderson and Woessner, 1992). Anderson and Woessner (1992) recommend that time steps be specified so that $\Delta t < \Delta l/V$ (or $C_o < 1.0$), which is equivalent to requiring that no solute be displaced by advection more than the distance across one grid cell or element during one time increment. Numerical error associated with the deviation of curves *C* or *D* (Figure 20.9) from the exact solution can be significant in some locations within the problem domain, although such errors tend to be minimal at the center of a front (relative concentration of 0.5).

In transport models, there may also be a grid-orientation effect in which the solute distribution, calculated for the same properties and boundary conditions, will vary somewhat depending on the angle of the flow relative to the grid. This phenomenon is largely related to the cross-product terms in the governing equation, and generally is not a serious source of error, but the model user should be aware of it.

20.6.5 Mass Balance

One measure of numerical accuracy is how well the model conserves mass. This can be measured by comparing the net fluxes calculated or specified in the model (e.g., inflow and sources minus outflow and sinks) with changes in storage (accumulation or depletion). Mass-balance calculations should always be performed and checked during the calibration procedure to help assess the numerical accuracy of the solution.

As part of these calculations, the hydraulic and chemical fluxes contributed by each distinct hydrologic component of the flow and transport model should be itemized separately to form hydrologic and chemical budgets for the system being modeled. The budgets are valuable assessment tools because they provide a measure of the relative importance of each component to the total budget.

Errors in the mass balance for flow models should generally be less than 0.1%. However, because the solute-transport equation is more difficult to solve numerically, the acceptable mass-balance error for a solute may be greater than for the fluid, but this will depend also on the nature of the numerical method implemented. Finite-difference and finite-element methods are inherently mass conservative, while some implementations of the method of characteristics and particle tracking approaches may not be (or their mass balance calculations themselves are only approximations). It must also be remembered that while a large mass-balance error provides evidence of a poor numerical solution, a perfect mass balance in itself does not and cannot prove that a true or accurate solution has been achieved or that the overall model is valid. That is, a perfect mass balance can be achieved if the model includes compensating errors. For example, the solutions C and D in Figure 20.9 that exhibit significant numerical dispersion or oscillatory behavior arise from solutions that show a near-perfect mass balance, but they are still wrong.

20.6.6 Sensitivity Tests

Assuming various values for given parameters also helps to achieve another objective of the calibration procedure, namely to determine the sensitivity of the model to factors that affect groundwater flow and transport and to errors and uncertainty in the data. Evaluating the relative importance of each factor helps determine which data must be defined most accurately and which data are already adequate or require only minimal further definition. If additional field data can be collected, such a sensitivity analysis helps in deciding which types of data are most critical and how to get the best information return on the costs of additional data collection. If additional data cannot be collected, then the sensitivity tests can help to assess the reliability of the model by demonstrating the effect of a given range of uncertainty or error in the input data on the output of the model. The relative sensitivities of the parameters that affect flow and transport will vary from problem to problem. Furthermore, the sensitivities may change over time as the stress regime imposed on a system evolves. Thus, one generalization is that a sensitivity analysis should be performed during the early stages of a model study.

The sensitivity of the solution to the grid design (or spacing), time-step criterion, nature and placement of boundary conditions, and other numerical parameters also should be evaluated, even if an inverse or regression modeling approach has been used. This step is frequently overlooked, but failure to do so may cause critical design flaws to remain undetected. For example, parameter-estimation models cannot evaluate the sensitivity to grid spacing or certain boundary conditions that are fixed in the model by the user. It is generally recommended that after a preliminary calibration has been achieved, the model should be rerun for the same stresses and properties using a finer grid, smaller time steps, and perhaps alternative boundary conditions. If such a test yields significantly different results, then the model should be recalibrated using design criteria that yield a more accurate numerical solution. If such a test yields no significant differences, then the coarser design is probably adequate for that particular problem.

20.6.7 Calibration Criteria

Model calibration may be viewed as an evolutionary process in which successive adjustments and modifications to the model are based on the results of previous simulations. The modeler must decide when sufficient adjustments have been made to the representation of parameters and processes and at some time accept the model as being adequately calibrated (or perhaps reject the model as being inadequate and seek alternative approaches). This decision is often based on a mix of subjective and objective criteria. The achievement of a best fit between values of observed and computed variables is a regression procedure and can be evaluated as such. That is, the residual errors should have a mean that approaches zero and the deviations should be minimized. Cooley (1977) discusses several statistical measures that can be used

to assess the reliability and "goodness of fit" of groundwater flow models. The accuracy tests should be applied to as many dependent variables as possible. The types of observed data that are most valuable for model calibration include head and concentration changes over space and time, and the quantity and quality of groundwater discharges from the aquifer.

While it is necessary to evaluate the accuracy of the model quantitatively, it is equally important to assure that the dependent variables that serve as a basis for the accuracy tests are reliable indicators of the computational power and accuracy of the model. For example, if a particular dependent variable was relatively insensitive to the governing parameters, then the existence of a high correlation between its observed and computed values would not necessarily be a reflection of a high level of accuracy in the overall model.

Similarly, caution must be exercised when the "observed data" contain an element of subjective interpretation. For example, matching an observed potentiometric surface or concentration distribution is sometimes used as a basis for calibrating groundwater models. However, a contoured surface is itself interpretive and can be a weak basis for model calibration because it includes a variability or error introduced by the contouring process, in addition to measurement errors present in the observed data at the specific points.

20.6.8 Predictions and Postaudits

As model calibration and parameter estimation are keyed to a set of historical data, the confidence in and reliability of the calibration process is proportional to the quality and comprehensiveness of the historical record. The time over which predictions are made with a calibrated model should also be related to, and limited by, the length of the historical record. A reasonable guideline is to predict only for a time comparable to the period that was matched.

The accuracy of a model's predictions is the best measure of its reliability. However, predictive accuracy can be evaluated only after the fact. Anderson and Woessner (1992) summarize several published studies in which the predictive accuracy of a deterministic groundwater model was evaluated several years after the prediction had been made. The results suggest that extrapolations into the future were rarely very accurate. Predictive errors often were related to having used a time period for history matching that was too short to capture an important element of the model or of the system, or to having an incomplete conceptual model. For example, processes and boundary conditions that are negligible or insignificant under the past and present stress regime may become nontrivial or even dominant under a different set of imposed stresses. Thus, a conceptual model founded on observed behavior of a groundwater system may prove to be inadequate in the future, when existing stresses are increased or new stresses are added. A major source of predictive error is sometimes attributable primarily to the uncertainty of future stresses, which is often controlled by demographic, political, economic, and (or) social factors. But if the range or probability of future stresses can be estimated, then the range or probability of future responses can be predicted. An encouraging trend is that many analysts are now attempting to place confidence bounds on predictions arising out of the uncertainty in parameter estimates. However, these confidence limits still would not bound errors arising from the selection of a wrong conceptual model or from problems in the numerical solution algorithms (Bredehoeft and Konikow, 1993).

If a model is to be used for prediction relating to a problem or system that is of continuing interest or significance to society, then field monitoring should continue and the model should be periodically postaudited, or recalibrated, to incorporate new information, such as changes in imposed stresses or revisions in the assumed conceptual model. A postaudit offers a means to evaluate the nature and magnitude of predictive errors, which may itself lead to a large increase in the understanding of the system and in the value of a subsequently revised model. Revised predictions can then be made with greater reliability.

20.6.9 Model Validation

It is natural for people who apply groundwater models, as well as those who make decisions based on model results, to want assurance that the model is valid. Groundwater models are embodiments of various scientific theories and hypotheses. Karl Popper (1959) argues that "as scientists we can never validate a hypothesis, only invalidate it." The same philosophy has been applied specifically to groundwater models (Konikow and Bredehoeft, 1992; Oreskes et al., 1994).

The criteria for labeling a model as validated are inherently subjective. In practice, validation is attempted through the same process that is typically and more correctly identified as calibration — that is, by comparing calculations with field or laboratory measurements. However, the nonuniqueness of model solutions means that a good comparison can be achieved with an inadequate or erroneous model. Also, because the definition of "good" is subjective, under the common operational definitions of validation, one competent and reasonable scientist may declare a model as validated while another may use the same data to demonstrate that the model is invalid. To the general public, proclaiming that a groundwater model is validated carries with it an aura of correctness that many modelers would not claim (Bredehoeft and Konikow, 1993). Because labeling a model as having been validated has very little objective or scientific meaning, such "certification" does little beyond instilling a false sense of confidence in such models. Konikow and Bredehoeft (1992) recommend that the term "validated" not be applied to groundwater models.

20.7 Overview of Representative Generic Models

A large number and variety of generic groundwater models are documented and available at the present time. Two widely used public domain models are explained in more detail as illustrative examples.

20.7.1 MODFLOW

One of the most popular and comprehensive deterministic groundwater models available today is the MODFLOW code of McDonald and Harbaugh (1988) and Harbaugh and McDonald (1996). This is actually a family of compatible codes that centers on an implicit finite-difference solution to the three-dimensional flow equation that was coded in FORTRAN in a modular style to allow and encourage the development of additional packages or modules that can be added on or linked to the original code. The basic model uses a block-centered finite-difference grid that allows variable spacing of the grid in three dimensions. Flow can be steady or transient. Layers can be simulated as confined, unconfined, or a combination of both. Aquifer properties can vary spatially and hydraulic conductivity (or transmissivity) can be anisotropic. Flow associated with external stresses, such as wells, areally distributed recharge, evapotranspiration, drains, and streams, can also be simulated through the use of specified head, specified flux, or head-dependent flux boundary conditions. The implicit finite-difference equations can be solved using either the strongly implicit procedure (SIP) or slice-successive overrelaxation (SSOR) methods. Newer packages offer several additional solution algorithms, including a preconditioned conjugate-gradient solver (Hill, 1990) and a direct solver (Harbaugh, 1995). Although the input and output systems of the program were designed to permit maximum flexibility, usability and ease of interpretation of model results can be enhanced by using one of several commercially available preprocessing and post-processing packages; some of these operate independently of MODFLOW, whereas others are directly integrated into reprogrammed and (or) recompiled versions of the MODFLOW code.

The pathline program MODPATH (Pollock, 1989, 1994) uses the results of the MODFLOW model and determines paths and travel times of water movement under steady-state and transient conditions. MODPATH uses a semianalytical particle-tracking scheme. The method assumes that each directional velocity component varies linearly within a grid cell in its own coordinate direction. MODPATH-PLOT is a graphics interface package that visually displays the results of MODPATH (Pollock, 1994).

The parameter-estimation package, MODFLOWP, can be used to estimate parameters (such as transmissivity, storage coefficient, leakance coefficients, recharge rates, evapotranspiration, and hydraulic head at constant-head boundaries) using nonlinear regression (Hill, 1992). Parameters are estimated by minimizing a weighted least-squares objective function by either the modified Gauss-Newton method or a conjugate-direction method. Data used to estimate parameters can include independent estimates of parameter values, observed heads or drawdowns, and observed gains or losses in streamflow. The MODFLOWP output includes statistics for analyzing the reliability of the estimated parameters and of the model.

A variety of other MODFLOW accessory codes, packages, and features are available. Most of these were developed by the U.S. Geological Survey (USGS) and are summarized by Appel and Reilly (1994); examples include coupled surface-water and groundwater flow, aquifer compaction, transient leakage from confining units, rewetting of dry cells, horizontal flow barriers, alternative interblock transmissivity conceptualizations, cylindrical flow to a well, a statistical processor, a data input program, and a program that calculates water budgets. Other packages have been developed by non-USGS sources to work with MODFLOW; one example is the advective-dispersive solute-transport model MT3D (Zheng, 1990).

20.7.2 MOC

The Method of Characteristics (MOC) model developed by Konikow and Bredehoeft (1978) simulates solute transport in flowing groundwater in two dimensions. The model has been extensively used since the mid-1970s and has been evolving through updates and improvements. The model computes changes in concentration over time caused by the processes of advective transport, hydrodynamic dispersion, mixing or dilution from fluid sources, and the following types of chemical reactions: first-order irreversible-rate reaction, such as radioactive decay; reversible equilibrium-controlled sorption with linear, Freundlich, or Langmuir isotherms; and reversible equilibrium-controlled ion exchange for monovalent or divalent ions. The model couples the groundwater flow equation with the solute-transport equation. The model uses a finite-difference approximation to the groundwater flow equation and the method of characteristics to solve the solute-transport equation. The model uses a particle tracking procedure to represent advective transport and an explicit finite-difference procedure to calculate concentration changes due to hydrodynamic dispersion.

The original model of Konikow and Bredehoeft (1978) was later revised by Goode and Konikow (1989) and Konikow et al. (1994). The model has also been used as the foundation for MOCDENSE (Sanford and Konikow, 1985), a model that can simulate two constituents in a density-dependent flow system. There are public-domain and commercial preprocessors available, including PREMOC (Granato et al., 1993). A three-dimensional version of the model (MOC3D) uses MODFLOW to simulate the flow system (Konikow et al., 1996).

20.8 Case Histories

A large number of documented examples of the application of groundwater models to a variety of hydrogeologic problems are available in the literature. Two case studies have been selected to help illustrate modeling philosophy and practice, including aspects of model conceptualization, model implementation, and interpretation of results.

20.8.1 Regional-Scale Flow in a Deep Confined Aquifer

The Powder River Basin of northeastern Wyoming and southeastern Montana contains large coal reserves that have not yet been fully developed. The future development of such energy resources in the Powder River Basin will be accompanied by increased demands for water, which is not abundantly available in this semiarid area. One plan had been formulated to construct a coal-slurry pipeline to transport coal out of the area; it would have required about 0.6 to 0.8 m^3/s of water. In the mid-1970s, a plan was

proposed to supply this water from up to 40 wells drilled about 1000 m into the Mississippian age Madison Limestone in Niobrara County, Wyoming. The Madison aquifer is an areally extensive carbonate rock system that underlies an area exceeding 260,000 km^2 in the northern Great Plains.

Concern that such relatively large groundwater withdrawals might cause significant water-level declines in the Madison aquifer, perhaps extending into adjacent states, as well as possibly causing decreases in streamflow and spring discharge in or near the outcrop areas, resulted in the need to predict the effects of the proposed large groundwater withdrawals on potentiometric levels, recharge, and discharge. Because the Madison aquifer lies at such great depths (from 300 to 5000 m) in most of the area, it is relatively undeveloped, and sufficient data are not available to define the head distribution and the hydraulic properties of the aquifer accurately and precisely. In light of this uncertainty, and as a prelude to a planned subsequent 5-year hydrogeologic investigation of the Madison aquifer, a preliminary, two-dimensional, finite-difference model of the aquifer was developed (Konikow, 1976). The objectives of the preliminary model study were to: (1) improve the conceptual model of groundwater flow in the aquifer system; (2) determine deficiencies in existing data, and help set priorities for future data collection by identifying the most sensitive parameters, assuming the model is appropriate; and (3) make a preliminary estimate of the regional hydrologic effects of the proposed well field (Konikow, 1976).

The results indicated that the aquifer can probably sustain the increased groundwater withdrawals, but that they probably would significantly lower the potentiometric surface in the Madison aquifer in a large part of the basin. Because of the great uncertainty in most of the parameters needed to represent the flow system, the model study and predictions were framed in terms of a sensitivity analysis. For example, Figure 20.10 shows drawdown predictions made for an area near the proposed well field for an assumed reasonable range of values for the storage and leakance coefficients (K_Z/m), where K_Z and m are the vertical hydraulic conductivity and the thickness, respectively, of the confining layer. The curves show that the range in plausible drawdowns, even after 1 year, is extremely large. The solutions also illustrate that sensitivities vary with time. At late times (about 100 years), there is no significant difference in drawdown for different values of S (simulations A, B, and C), and at early times (up to about 0.1 years) the drawdown is about the same for all values of leakance at a given value of S (simulations B, D, E, and F).

This preliminary model analysis helped in formulating an improved conceptual model of the Madison aquifer. For example, the important influences of temperature differences and aquifer discontinuities on groundwater flow were recognized and documented (see Konikow, 1976). Because the discrepancies between observed heads and those calculated with the earliest preliminary models did not appear to be

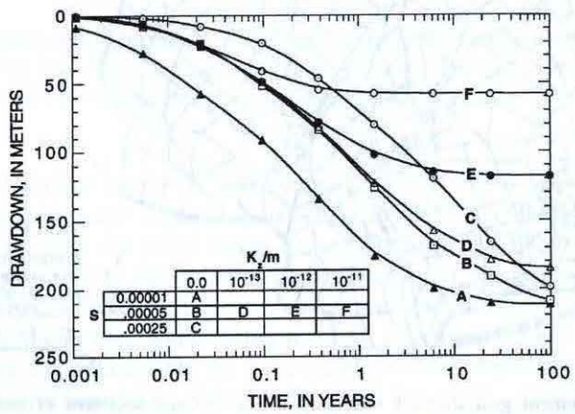

FIGURE 20.10 Time-drawdown curves for model node located near proposed well field to pump groundwater from the Madison Limestone aquifer. (Adapted from Konikow, L. F. 1976. Preliminary digital model of ground-water flow in the Madison group, Powder River basin and adjacent areas, Wyoming, Montana, South Dakota, North Dakota, and Nebraska. U.S. Geol. Survey Water-Res. Inv. 63-75.)

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distributed randomly, it was thought that data uncertainty was not the only source of error. Although it could be argued that the importance of these influences could have been (or should have been) recognized on the basis of hydrogeologic principles without the use of a simulation model, the fact is that none of the earlier published studies of this aquifer system indicated that these factors were of major significance. The improvement over earlier studies arose from the quantitative hypothesis-testing role of the model; the nature of the inconsistencies between observed head distributions and those calculated using the initial estimates of model parameters helped direct the investigators toward testing hypotheses that would resolve or minimize the inconsistencies with only a small increment of added complexity. The demonstrated high sensitivity of drawdown to the leakance coefficient emphasized the need to reevaluate the system in a true three-dimensional framework so as to represent vertical components of flow more accurately, which was done in several subsequent studies (for example, see Downey and Weiss, 1980; Woodward-Clyde Consultants, 1981).

Cooley et al. (1986) applied a nonlinear-regression groundwater flow model to this same aquifer system. Their two-dimensional model was based on a Galerkin finite-element discretization scheme. The finite-element grid and boundary conditions are shown in Figure 20.11. The grid was designed to be finer where more data were available and (or) where hydraulic gradients are relatively steep. Regression analysis was used to estimate parameters, including intrinsic permeabilities of the main aquifer and separate lineament zones, discharges from eight major springs, and specified heads on the model boundaries. The regression approach also yielded statistical measures of the reliability of those parameter estimates. Analysis by Cooley et al. (1986) tends to confirm the existence of lineament zones, which appear to exert a strong influence upon the flow and head distribution in the Madison aquifer.

Thus, results from a variety of models were used to understand the sensitivity of the response of the conceptualized Madison aquifer to changes in simulated aquifer parameters. From these sensitivity analyses, improved predictions of aquifer responses were made, and the confidence in the predictions were assessed.

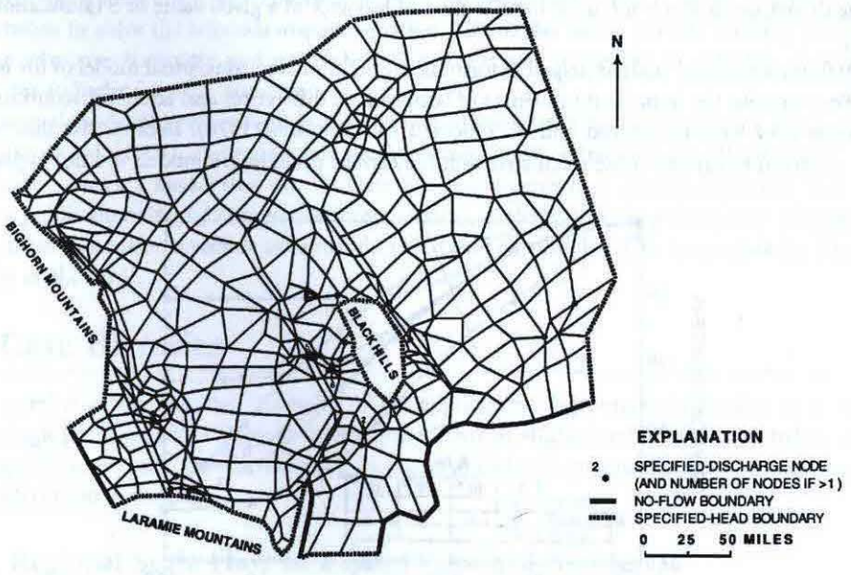

FIGURE 20.11 Finite-element grid showing boundary conditions and locations of specified-discharge points. (Adapted from Cooley, R. L., Konikow, L. F., and Naff, R. L. 1986. Nonlinear-regression groundwater flow modeling of a deep regional aquifer system. *Water Resour. Res.* 10(3):546-562.)

20.8.2 Local-Scale Flow and Transport in a Shallow Unconfined Aquifer

Reilly et al. (1994) combined the application of environmental tracers and deterministic numerical modeling to analyze and estimate recharge rates, flow rates, flow paths, and mixing properties of a shallow groundwater system near Locust Grove, in eastern Maryland. The study was undertaken as part of the U.S. Geological Survey's National Water Quality Assessment Program to provide flow paths and travel time estimates to be used in understanding and interpreting water-quality trends in monitoring wells and stream base flows. The study area encompassed about 2.6×10^7 m^2 of mostly agricultural land on the Delmarva Peninsula. The surficial aquifer includes unconsolidated permeable sands and gravel that range in thickness from less than 6 m to more than 20 m. This surficial aquifer is underlain by relatively impermeable silt and clay deposits, which form a confining unit.

In this study, chlorofluorocarbons (CFCs) and tritium were analyzed from a number of water samples collected from observation wells to estimate the age of groundwater at each sampling location and depth. Because errors and uncertainty are associated with estimates of age based on environmental tracers, just as errors and uncertainty are associated with deterministic models of groundwater flow and transport, the authors applied a feedback or iterative process based on comparisons of independent estimates of travel time. Their approach is summarized and outlined in Figure 20.12. Each task shown was designed to improve either the estimates of parameters or the conceptualization of the system.

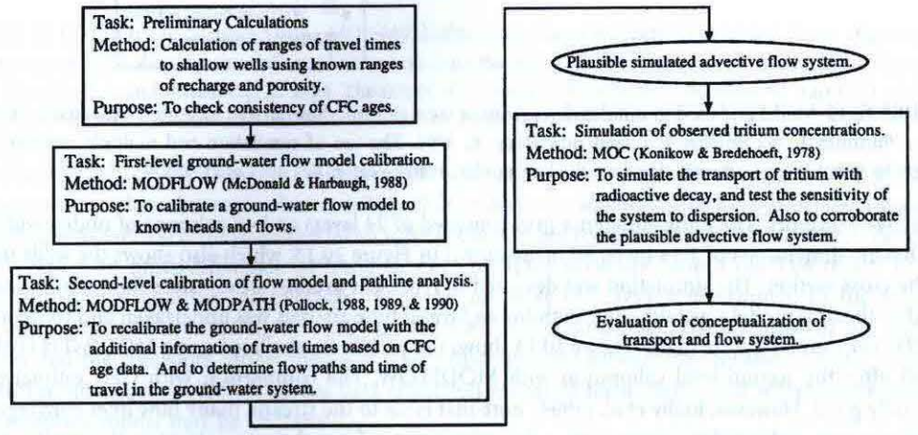

FIGURE 20.12 Flow diagram of the steps taken to quantify the flow paths in the Locust Grove, Maryland, groundwater flow system. (Adapted from Reilly, T. E., Plummer, L. N., Phillips, P. J., and Busenberg, E. 1994. The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour. Res.* 30(2):421-433.)

The preliminary calculations (first task) were used to set bounds on the plausibility of the results of the more complex simulations and chemical analyses. The first-level calibration of a groundwater flow model (second task) provided the initial system conceptualization. The third task was a second-level calibration and analysis involving simulation of advective transport, which provided quantitative estimates of flow paths and time of travel to compare with those obtained from the CFC analyses. The fourth task involved the application of a solute-transport model to simulate tritium concentrations in the groundwater flow system as influenced by the processes of advection, dispersion, radioactive decay, and time-varying input (source concentration) functions.

The sampling wells were located approximately along an areal flow line, and a two-dimensional cross-sectional model was developed for the simulation of processes occurring along this flow line. The MODFLOW model (McDonald and Harbaugh, 1988) was used to simulate groundwater flow and

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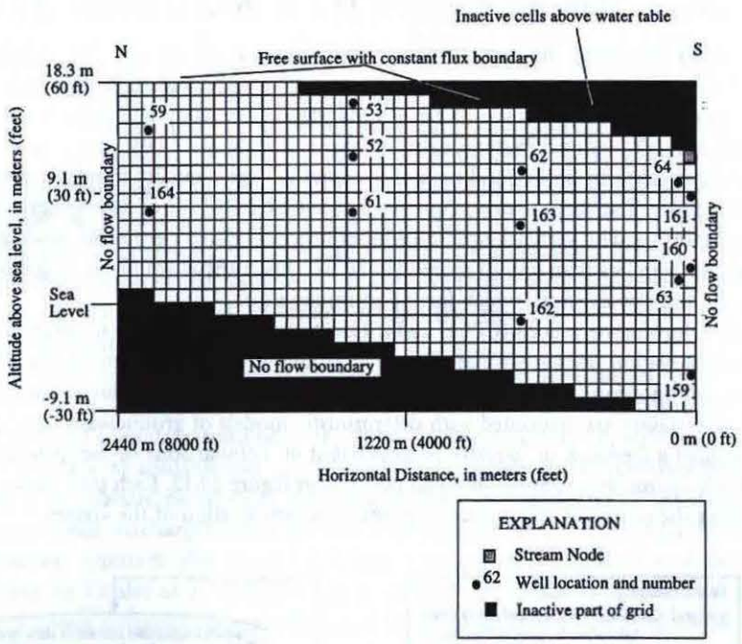

FIGURE 20.13 Model grid used to simulate Locust Grove cross section, showing well locations. (Adapted from Reilly, T. E., Plummer, L. N., Phillips, P. J., and Busenberg, E. 1994. The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour. Res.* 30(2):421-433.)

advective transport. The finite-difference grid consisted of 24 layers and 48 columns of nodes, with each cell having dimensions of 1.14 by 50.80 m, as shown in Figure 20.13, which also shows the wells that lie in the cross section. The simulation was designed to represent average steady-state flow conditions.

After the flow model was calibrated, pathline and travel time analysis was undertaken and comparisons to CFC age estimates were made. Figure 20.14 shows the pathlines calculated using MODPATH (Pollock, 1989) after the second-level calibration with MODFLOW. The comparison with CFC estimates was generally good. However, Reilly et al. (1994) note that close to the stream, many flow lines converge, and the convergence of pathlines representing the entire range of travel times present in the aquifer causes waters of different ages to be relatively near each other. Thus, at the scale and grid spacing of the model, in the area near the stream the convergent flow lines cannot be readily differentiated in the model and the locations of individual well screens cannot be accurately represented directly under the stream. After the second-level calibration, the root mean squared error between the simulated ages and the CFC ages for the 10 wells farthest from the stream (i.e., excluding wells 159, 160, and 161) was 3.4 years.

Tritium concentrations of recharge waters have varied considerably over the last 40 years. Thus, the time of travel would not always be readily apparent from the tritium concentration in a water sample. Also, mixing of waters recharged during periods of these relatively sharp changes of input concentrations can make the interpretation of time of travel from tritium concentrations even more uncertain. Thus, the investigators simulated solute transport of tritium within the system using a model that accounts for mixing (dispersion), radioactive decay, and transient input functions, which also allowed a further evaluation of consistency with the results of the previous flow and advective transport model. They applied the MOC solute-transport model of Konikow and Bredehoeft (1978) and Goode and Konikow (1989) for this purpose.

The results of the simulation of the tritium distribution assuming (1) no dispersion and (2) α_L of 0.15 m and α_T of 0.015 m are shown in Figure 20.15. The limiting case simulation of no dispersion yielded acceptable results and was used as the best estimate of the tritium distribution in November

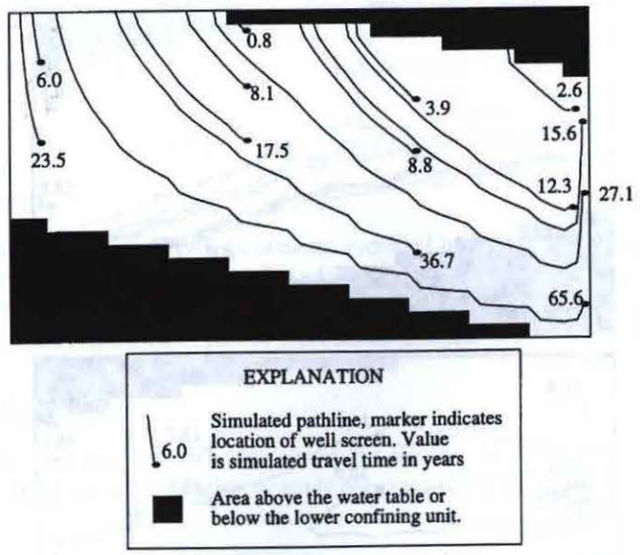

FIGURE 20.14 Pathlines (calculated using MODPATH after second-level calibration) in Locust Grove cross section to observation wells showing time of travel (in years) from the water table. (Adapted from Reilly, T. E., Plummer, L. N., Phillips, P. J., and Busenberg, E. 1994. The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour. Res.* 30(2):421-433.)

1990 (Reilly et al., 1994). This case reproduces the sharp concentration gradients required to reproduce the low tritium values that were observed. The MOC model was advantageous for this problem because it minimizes numerical dispersion and it can solve the governing equations for α_L of 0.0, which transport models based on finite-difference or finite-element methods generally cannot do. The results of the solute-transport simulation are consistent with the advective flow system determined by the second-level calibration and thus strengthen the case for the conceptual model. The coupling of the tritium analyses and the transport model indicates where discrepancies between the measured and simulated concentrations occur, where additional data collection would be most useful, and where refinement of the conceptual model may be warranted.

This case study illustrates that environmental tracers and numerical simulation methods in combination are effective tools that complement each other and provide a means to estimate the flow rate and path of water moving through a groundwater system. Reilly et al. (1994) found that the environmental tracers and numerical simulation methods also provide a "feedback" that allows a more objective estimate of the uncertainties in the estimated rates and paths of movement. Together the two methods enabled a coherent explanation of the flow paths and rates of movement while identifying weaknesses in the understanding of the system that require additional data collection and refinement of conceptual models of the groundwater system.

20.9 Available Groundwater Models

A large number of generic deterministic groundwater models, based on a variety of numerical methods and a variety of conceptual models, are available. The selection of a numerical method or generic model for a particular field problem depends on several factors, including accuracy, efficiency/cost, and usability. The first two factors are related primarily to the nature of the field problem, availability of data, and scope or intensity of the investigation. The usability of a method may depend partly on the mathematical background of the modeler, as it is preferable for the model user to understand the nature of the numerical methods implemented in a code. It may be necessary to modify and adapt the program to the specific

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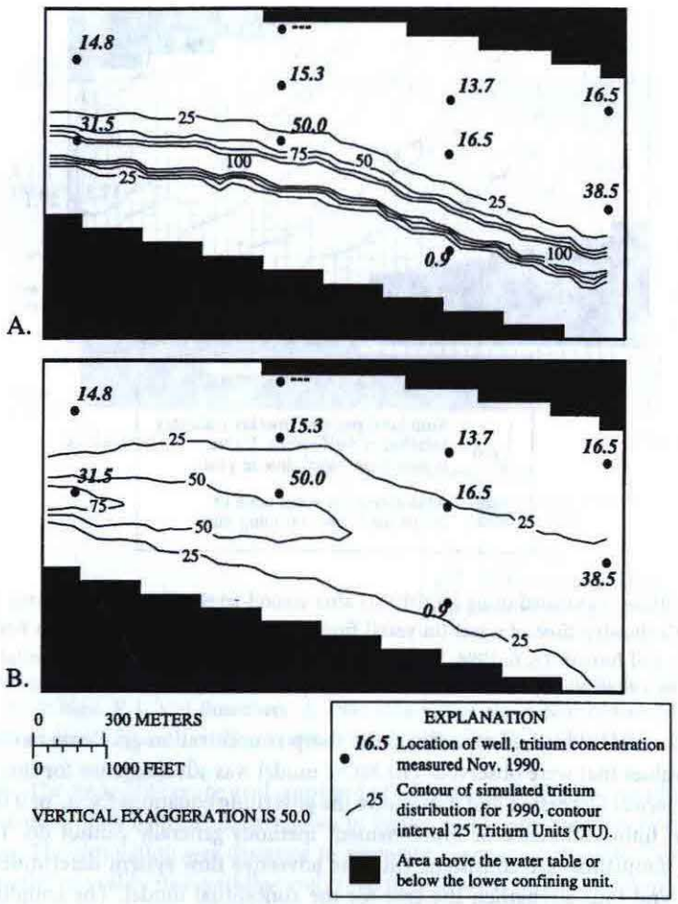

FIGURE 20.15 Simulated tritium distribution at the end of 1990: (A) with dispersivity $\alpha_L = 0.0$ m and $\alpha_T = 0.0$ m, and (B) with dispersivity $\alpha_L = 0.15$ m and $\alpha_T = 0.015$ m. Contour interval 25 tritium units (TU). Measured concentrations from samples obtained from wells in November 1990 are given for their location in bold italics. (Adapted from Reilly, T. E., Plummer, L. N., Phillips, P. J., and Busenberg, E. 1994. The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour. Res.* 30(2):421-433.)

problem of interest, and this can sometimes require modifications to the source code. In selecting a model that is appropriate for a particular application, it is most important to choose one that incorporates the proper conceptual model; one must avoid force fitting an inappropriate model to a field situation solely because of the model's convenience, availability, or familiarity to the user. Usability is also enhanced by the availability of preprocessing and postprocessing programs or features, and by the availability of comprehensive yet understandable documentation.

A number of surveys of available models have been published in recent years (Appel and Reilly, 1994; Van der Heijde et al., 1985). Van der Heijde et al. (1985) report on an international survey of 399 models, of which 206 had been documented at that time. This was a significant increase from the 245 models available for a similar review 5 years earlier. Appel and Reilly (1994) summarize the nature and availability of 89 groundwater flow and quality models produced by and available from the U.S. Geological Survey. Anderson et al. (1992), in their review of groundwater models, list 19 separate software distributors and provide brief descriptions of several codes. The International Ground Water Modeling Center, Golden, CO, (see internet address in *For Further Information*) maintains a clearinghouse and distribution center for groundwater simulation models.

A large number of public and private organizations distribute public domain and (or) proprietary software for groundwater modeling. A growing availability of models is also occurring on the internet (see *For Further Information* for some examples). Some internet sites allow computer codes to be downloaded at no cost, while other sites provide catalog information, demonstrations, and pricing information.

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For Further Information

Textbooks and examples of good reports on site-specific models are provided as starting points for readers who would like to obtain more information or study representative applications.

Textbooks

Anderson and Woessner (1992) present an overview of applied groundwater flow and advective transport modeling.

Zheng and Bennett (1995) present an overview of the theory and practice of contaminant transport modeling.

Examples of Reports on Site-Specific Models

Comprehensive reports on site-specific models provide insight into applied groundwater simulation. A few examples from the work of the U.S. Geological Survey are provided below. Obviously, this list is not inclusive, and many other reports could have been listed.

Regional Flow Models

Kernodle et al. (1995) describe a three-dimensional flow model of the Albuquerque Basin in New Mexico.

Fleck and Vroblesky (1996) describe the application of a three-dimensional groundwater flow model to a coastal plain system in the northeastern U.S.

Local Flow Model

Masterson and Barlow (1994) used a two-step approach to simulate a saltwater–freshwater system.

Local Radial-Flow Model

Lindner and Reilly (1983) used a finite-element radial flow model to analyze aquifer tests on Long Island, New York.

Local Advective-Transport Model

Barlow (1994) examined contributing areas to public-supply wells at Cape Cod, Massachusetts.

Solute-Transport Model

LeBlanc (1984) documented a two-dimensional simulation of a 6-km-long sewage plume at Cape Cod, Massachusetts.

Lambert (1996) used a three-dimensional model to simulate a contaminant plume in an approximately 480-km^2 area in Utah.

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Model Calibration

Masterson et al. (1996) used particle tracking and contaminant plumes to improve calibration of a three-dimensional flow model.

Yager (1997) used a parameter-estimation model (MODFLOWP) to help calibrate a three-dimensional flow model for a fractured dolomite aquifer system.

Internet

A number of sites on the World Wide Web provide compendia of codes and sources of information about groundwater modeling, as well as providing links to other websites related to groundwater modeling. Many of these sites allow codes to be downloaded. Examples of several groundwater-oriented home page locations are: **http://www.ems.psu.edu/Hydrogeologist/**, **http://www.et.byu.edu/~asce-gw/**, **http://www.mines.edu/igwmc/**, and **http://www.ibmpcug.co.uk/~bedrock/gsd/**. Also, many of the U.S. Geological Survey public domain codes are available from the "USGS Water Resources Applications Software" link on the USGS Water Resources Information Home page at: **http://water.usgs.gov/**.

References

Anderson, M. P. 1984. Movement of contaminants in groundwater: Groundwater transport — Advection and dispersion, in *Groundwater Contamination.* National Academy Press, Washington, D.C., 37-45.

Anderson, M. P., Ward, D. S., Lappala, E. G., and Prickett, T. A. 1992. Computer models for subsurface water, in *Handbook of Hydrology.* Ed. D.R. Maidment, McGraw-Hill, New York, 22.1-22.34.

Anderson, M. P. and Woessner, W. W. 1992. *Applied Groundwater Modeling.* Academic Press, San Diego.

Appel, C. A. and Reilly, T. E. 1994. *Summary of Computer Programs Produced by the U.S. Geological Survey for Simulation of Ground-Water Flow and Quality — 1994.* U.S. Geol. Survey Circular 1104.

Barlow, P. M. 1994. Particle-tracking analysis of contributing areas of public-supply wells in simple and complex flow systems, Cape Cod, Massachusetts. U.S. Geol. Survey Open-File Rept. 93-159.

Bear, J. 1979. *Hydraulics of Groundwater.* McGraw-Hill, New York.

Bear, J. and Verruijt, A. 1987. *Modeling Groundwater Flow and Pollution.* Reidel Publishing Co., Dordrecht, The Netherlands.

Bennett, G. D. 1976. *Introduction to Ground-Water Hydraulics: A Programmed Text for Self-Instruction.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 3, Ch. B2.

Bredehoeft, J. D. and Konikow, L. F. 1993. Ground-water models: Validate or invalidate. *Ground Water.* 31(2):178-179.

Cooley, R. L. 1977. A method of estimating parameters and assessing reliability for models of steady state groundwater flow, 1., Theory and numerical properties. *Water Resour. Res.* 13(2):318-324.

Cooley, R. L. 1992. *A Modular Finite-Element Model (MODFE) for Areal and Axisymmetric Ground-water-Flow Problems, Part 2: Derivation of Finite-Element Equations and Comparisons with Analytical Solutions,* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 6, Ch. A4.

Cooley, R. L., Konikow, L. F., and Naff, R. L. 1986. Nonlinear-regression groundwater flow modeling of a deep regional aquifer system. *Water Resour. Res.* 10(3):546-562.

Domenico, P. A. and Robbins, G. A. 1984. A dispersion scale effect in model calibrations and field tracer experiments, *J. Hydrol.* 70:123-132.

Domenico, P. A. and Schwartz, F. W. 1990. *Physical and Chemical Hydrogeology.* John Wiley & Sons, New York.

Downey, J. S. and Weiss, E. J. 1980. Preliminary data set for three-dimensional digital model of the Red River and Madison aquifers. U.S. Geol. Survey Open-File Rept. 80-756.

Fleck, W. B. and Vroblesky, D. A. 1996. Simulation of ground-water flow of the coastal plain aquifers in parts of Maryland, Delaware, and the District of Columbia. U.S. Geol. Survey Prof. Paper 1404-J.

Franke, O. L. and Reilly, T. E. 1987. The effects of boundary conditions on the steady-state response of three hypothetical groundwater systems — Results and implications of numerical experiments. U.S. Geol. Survey Water-Supply Paper 2315.

Franke, O. L., Reilly, T. E., and Bennett, G. D. 1987. *Definition of Boundary and Initial Conditions in the Analysis of Saturated Ground-Water Flow Systems — An Introduction.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 3, Ch. B5.

Freyberg, D. L. 1988. An exercise in ground-water model calibration and prediction. *Ground Water.* 26(3):350-360.

Garder, A. O., Peaceman, D. W., and Pozzi, A. L. 1964. Numerical calculation of multidimensional miscible displacement by the method of characteristics. *Soc. Petroleum Eng. J.* 4(1):26-36.

Gelhar, L. W. 1993. *Stochastic Subsurface Hydrology.* Prentice Hall, Englewood Cliffs, NJ.

Gelhar, L. W., Welty, C., and Rehfeldt, K. R. 1992. A critical review of data on field-scale dispersion in aquifers. *Water Resour. Res.* 28(7):1955-1974.

Goode, D. J. and Appel, C. A. 1992. Finite-difference interblock transmissivity for unconfined aquifers and for aquifers having smoothly varying transmissivity. U.S. Geol. Survey Water-Res. Inv. Rept. 92-4124.

Goode, D. J. and Konikow, L. F. 1989. Modification of a method-of-characteristics solute-transport model to incorporate decay and equilibrium-controlled sorption or ion exchange. U.S. Geol. Survey Water-Res. Inv. Rept. 89-4030.

Goode, D. J. and Konikow, L. F. 1990. Apparent dispersion in transient groundwater flow. *Water Resour. Res.* 26(10):2339-2351.

Granato, G. E., Konikow, L. F., and Srinivasan, P. 1993. PREMOC version 4.0, A preprocessor for the two-dimensional method of characteristics (MOC) solute-transport model. International Ground Water Modeling Center, Golden, CO, Report IGWMC — FOS 23.

Grove, D. B. 1976. Ion exchange reactions important in groundwater quality models, in *Advances in Groundwater Hydrology,* Am. Water Res. Assoc., Minneapolis, 409-436.

Haitjema, H. M. 1995. *Analytic Element Modeling of Groundwater Flow.* Academic Press, San Diego.

Harbaugh, A. W. 1995. Direct solution package based on alternating diagonal ordering for the U.S. Geological Survey modular finite-difference ground-water flow model. U.S. Geol. Survey Open-File Rept. 95-288.

Harbaugh, A. W. and McDonald, M. G. 1996. User's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model. U.S. Geol. Survey Open-File Report 96-485.

Hill, M. C. 1990. Preconditioned Conjugate-Gradient 2 (PCG2) — A computer program for solving ground-water flow equations. U.S. Geol. Survey Water-Res. Inv. Rept. 90-4048.

Hill, M. C. 1992. A computer program (MODFLOWP) for estimating parameters of a transient, three-dimensional, ground-water flow model using nonlinear regression. U.S. Geol. Survey Open-File Rept. 91-484.

Huebner, K. H. 1975. *The Finite Element Method for Engineers.* John Wiley & Sons, New York.

Huyakorn, P. S. and Pinder, G. F. 1983. *Computational Methods in Subsurface Flow.* Academic Press, New York.

Javandel, I., Doughty, D., and Tsang, C. -F. 1984. *Groundwater Transport: Handbook of Mathematical Models.* Am. Geophysical Union, Water Res. Monograph 10.

Kernodle, J. M., McAda, D. P., and Thorn, C. R. 1995. Simulation of ground-water flow in the Albuquerque Basin, central New Mexico, 1901-1994, with projections to 2020. U.S. Geol. Survey Water-Res. Inv. Rept. 94-4251.

Kipp, K. L. Jr. 1987. HST3D: A computer code for simulation of heat and solute transport in three-dimensional ground-water flow systems. U.S. Geol. Survey Water-Res. Inv. Rept. 86-4095.

Konikow, L. F. 1976. Preliminary digital model of ground-water flow in the Madison group, Powder River basin and adjacent areas, Wyoming, Montana, South Dakota, North Dakota, and Nebraska. U.S. Geol. Survey Water-Res. Inv. 63-75.

Konikow, L. F. 1996. Numerical models of groundwater flow and transport, in *Manual on Mathematical Models in Isotope Hydrogeology.* International Atomic Energy Agency, Vienna.

Konikow, L. F. and Bredehoeft, J. D. 1978. *Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 7, Ch. C2.

Konikow, L. F. and Bredehoeft, J. D. 1992. Ground-water models cannot be validated. *Advances in Water Resources.* 15(1):75-83.

Konikow, L. F. and Grove, D. B. 1977. Derivation of equations describing solute transport in ground water. U.S. Geological Survey Water-Res. Inv. Rept. 77-19.

Konikow, L. F., Goode, D. J., and Hornberger, G. Z. 1996. A three-dimensional method-of-characteristics solute-transport model (MOC3D). U.S. Geol. Survey Water-Res. Inv. Rept. 96-4267.

Konikow, L. F., Granato, G. E., and Hornberger, G. Z. 1994. User's guide to revised method-of-characteristics solute-transport model (MOC—Version 3.1). U.S. Geol. Survey Water-Res. Inv. Rept. 94-4115.

Konikow, L. F. and Mercer, J. M. 1988. Groundwater flow and transport modeling, *J. Hydrol.* 100(2):379-409.

Lambert, P. M. 1996. Numerical simulation of the movement of sulfate in ground water in southwestern Salt Lake Valley, Utah. Tech. Pub. No. 110-D, Utah Dept. of Natural Resources, Salt Lake City, UT.

LeBlanc, D. R. 1984. Digital modeling of solute transport in a plume of sewage-contaminated ground water, in *Movement and Fate of Solutes in a Plume of Sewage Contaminated Ground Water, Cape Cod, Massachusetts.* U.S. Geological Survey Toxic Waste Ground-Water Contamination Program, ed. D.R. LeBlanc. P. 11-45. U.S. Geol. Survey Open-File Rept. 84-475.

Lindner, J. B. and Reilly, T. E. 1983. Analysis of three tests of the unconfined aquifer in southern Nassau County, Long Island, New York. U.S. Geol. Survey Water-Res. Inv. Rept. 82-4021.

Masterson, J. P. and Barlow, P. M. 1994. Effects of simulated ground-water pumping and recharge on ground-water flow in Cape Cod, Martha's Vineyard, and Nantucket Island Basins, Massachusetts. U.S. Geol. Survey Open-File Rept. 94-316.

Masterson, J. P., Walter, D. A., and Savoie, J. 1996. Use of particle tracking to improve numerical model calibration and to analyze ground-water flow and contaminant migration, Massachusetts Military Reservation, western Cape Cod, Massachusetts. U.S. Geol. Survey Open-File Rept. 96-214.

McDonald, M. G. and Harbaugh, A. W. 1988. *A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model.* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 6, Ch. A1.

Mercer, J. W. and Faust, C. R. 1981. *Ground-Water Modeling.* Natl. Water Well Assoc., Worthington, Ohio.

Oreskes, N., Shrader-Frechette, K., and Belitz, K. 1994. Verification, validation, and confirmation of numerical models in the earth sciences. *Science.* 263:641-646.

Peaceman, D. W. 1977. *Fundamentals of Numerical Reservoir Simulation.* Elsevier, Amsterdam.

Pollock, D. W. 1988. Semianalytical computation of path lines for finite-difference models. *Ground Water.* 26(6):743-750.

Pollock, D. W. 1989. Documentation of computer programs to compute and display pathlines using results from the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model. U.S. Geol. Survey Open-File Rept. 89-381.

Pollock, D. W. 1994. User's guide for MODPATH/MODPATH-PLOT, version 3: A particle tracking post processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model. U.S. Geol. Survey Open-File Rept. 94-464.

Popper, Sir Karl. 1959. *The Logic of Scientific Discovery.* Harper and Row, New York.

Prickett, T. A., Naymik, T. G., and Lonnquist, C. G. 1981. A "random-walk" solute transport model for selected groundwater quality evaluations. Ill. State Water Survey Bulletin 65.

Reddell, D. L. and Sunada, D. K. 1970. Numerical simulation of dispersion in groundwater aquifers. Colorado State University, Ft. Collins, Hydrology Paper 41.

Reilly, T. E., Franke, O. L., Buxton, H. T., and Bennett, G. D. 1987. A conceptual framework for ground-water solute-transport studies with emphasis on physical mechanisms of solute movement. U.S. Geol. Survey Water-Res. Inv. Rept. 87-4191.

Reilly, T. E., Plummer, L. N., Phillips, P. J., and Busenberg, E. 1994. The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour. Res.* 30(2):421-433.

Remson, I., Hornberger, G. M., and Molz, F. J. 1971. *Numerical Methods in Subsurface Hydrology,* John Wiley & Sons, New York.

Sanford, W. E. and Konikow, L. F. 1985. A two-constituent solute-transport model for ground water having variable density. U.S. Geol. Survey Water-Res. Inv. Rept. 85-4279.

Ségol, G. 1994. *Classic Groundwater Simulations: Proving and Improving Numerical Models.* PTR Prentice Hall, Englewood Cliffs, NJ.

Smith, L. and Schwartz, F. W. 1980. Mass transport, 1, A stochastic analysis of macroscopic dispersion. *Water Resour. Res.* 16(2):303-313.

Swedish Nuclear Power Inspectorate. 1987. The International HYDROCOIN Project—Background and Results, OECD, Paris.

Torak, L. J. 1993. A modular finite-element model (MODFE) for areal and axisymmetric ground-water-flow problems, Part 1: Model description and user's manual. Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 6, Ch. A3.

Van der Heijde, P. K. M., Bachmat, Y., Bredehoeft, J. D., Andrews, B., Holtz, D., and Sebastian, S. 1985. *Groundwater Management: The Use Of Numerical Models,* American Geophys. Union, Washington, D.C., Water Res. Monograph 5 (2nd Ed.).

Voss, C. I. 1984. SUTRA — Saturated Unsaturated Transport — A finite-element simulation model for saturated-unsaturated fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport. U.S. Geol. Survey Water-Res. Invest. Rep. 84-4369.

Wang, J. F. and Anderson, M. P. 1982 (reprinted, 1995). *Introduction to Groundwater Modeling,* Academic Press, San Diego.

Wexler, E. J. 1992. *Analytical Solutions for One-, Two-, and Three-Dimensional Solute Transport in Ground-Water Systems with Uniform Flow,* Techniques of Water-Res. Invests. of the U.S. Geol. Survey, Book 3, Ch. B7.

Woodward-Clyde Consultants. 1981. Well-field hydrology technical report for the ETSI coal slurry pipeline project. Bureau of Land Management, Washington, D.C.

Yager, R. M. 1997. Simulated three-dimensional ground-water flow in the Lockport Group, a fractured dolomite aquifer near Niagara Falls, New York. U.S. Geol. Survey Water-Supply Paper 2487.

Yeh, W. W.-G. 1986. Review of parameter identification procedures in groundwater hydrology: The inverse problem. *Water Resour. Res.* 22(1):95-108.

Zheng, C. 1990. *MT3D: A Modular Three-Dimensional Transport Model.* S.S. Papadopulos and Associates, Inc., Bethesda, MD.

Zheng, C. and Bennett, G. D. 1995. *Applied Contaminant Transport Modeling,* Van Nostrand–Reinhold, New York.

Zienkiewicz, O. C. 1971. *The Finite Element Method in Engineering Science.* McGraw-Hill, London.

Glossary

Analytical Model A closed-form exact mathematical solution which is continuous in space and time.
Conceptual Model A hypothesis for how a system or process operates.
Deterministic Model A mathematical model based on conservation of mass, momentum, and energy.
Discretization The process of representing a continuous system by a set of discrete blocks, cells, or elements.
Generic Model The computer code used to solve one or more partial differential equations.
Mathematical Model A set of equations, which include mathematical variables, constants, and coefficients, that represents relevant processes.
Model A representation of a real system or process.

Numerical Model An approximate solution of a differential equation obtained by replacing the continuous variables with a set of discrete variables defined at grid blocks, cells, or nodes.

Site-Specific Model A numerical model with the parameters (such as hydraulic conductivity, dispersivity, etc.), boundary conditions, and grid dimensions of the generic model specified to represent a particular geographical area.

21

The Role of Geographical Information Systems in Groundwater Engineering

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Resource 21

21.1 Introduction to Geographic Information Systems (GIS)

Geographic Information Systems (GIS) have become important tools in efficiently solving many problems in which spatial data are important. Natural resources and environmental concerns, including groundwater, have benefited greatly from the use of GIS. This chapter provides a brief introduction to GIS and some of its applications in addressing groundwater issues.

21.1.1 Overview of GIS

GIS have evolved rapidly in the last decade, becoming powerful computer tools for varied applications ranging from sophisticated analysis and modeling of spatial data to simple inventory and management.

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